```
d his ful

     (FILE 'HOME' ENTERED AT 17:20:35 ON 31 AUG 2005)

     FILE 'REGISTRY' ENTERED AT 17:20:39 ON 31 AUG 2005
L1             STRUCTURE UPLOADED
L2          17 SEA SSS FUL L1
               D L2 1-17 ED

     FILE 'HCAPLUS' ENTERED AT 17:21:29 ON 31 AUG 2005
L3           3 SEA PLU=ON  L2
               D L3 1-3 IBIB

     FILE 'REGISTRY' ENTERED AT 17:46:40 ON 31 AUG 2005
L4             STRUCTURE UPLOADED
L5          20 SEA SSS FUL L4

     FILE 'HCAPLUS' ENTERED AT 17:47:06 ON 31 AUG 2005
L6           1 SEA PLU=ON  L5
               D L6


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   30 AUG 2005  HIGHEST RN 862155-39-3
     DICTIONARY FILE UPDATES:  30 AUG 2005  HIGHEST RN 862155-39-3

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

       Please note that search-term pricing does apply when
       conducting SmartSELECT searches.

     ************************************************************
     *                                                          *
     * The CA roles and document type information have been removed from *
     * the IDE default display format and the ED field has been added,   *
     * effective March 20, 2005.  A new display format, IDERL, is now    *
     * available and contains the CA role and document type information. *
     *                                                          *
     ************************************************************

     Structure search iteration limits have been increased.  See HELP SLIMITS
     for details.

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     to the file summary sheet on the web at:
     http://www.cas.org/ONLINE/DBSS/registryss.html

     FILE HCAPLUS

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```

FILE COVERS 1907 - 31 Aug 2005 VOL 143 ISS 10
FILE LAST UPDATED: 30 Aug 2005 (20050830/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

10/762,582

```
=> d his ful

     (FILE 'HOME' ENTERED AT 14:21:20 ON 31 AUG 2005)

     FILE 'REGISTRY' ENTERED AT 14:21:26 ON 31 AUG 2005
L1                STRUCTURE UPLOADED
L2             50 SEA SSS SAM L1
L3           2305 SEA SSS FUL L1
L4                STRUCTURE UPLOADED
L5           2199 SEA SUB=L3 SSS FUL L4
L6                STRUCTURE UPLOADED
L7           2199 SEA SUB=L5 SSS FUL L6
L8                STRUCTURE UPLOADED
L9           2107 SEA SUB=L7 SSS FUL L8
L10            92 SEA PLU=ON  L7 NOT L9

     FILE 'HCAPLUS, USPATFULL, TOXCENTER' ENTERED AT 14:28:20 ON 31 AUG 2005
L11           281 SEA PLU=ON  L10
L12           259 DUP REM L11 (22 DUPLICATES REMOVED)
                      ANSWERS '1-237' FROM FILE HCAPLUS
                      ANSWERS '238-259' FROM FILE USPATFULL

     FILE 'HCAPLUS, USPATFULL' ENTERED AT 14:28:56 ON 31 AUG 2005
L13           259 SEA PLU=ON  L12
L14           253 SEA PLU=ON  L13 AND (PD<20030129 OR PRD<20030129)
L15           243 SEA PLU=ON  L14 AND PD<20020129
L16           243 DUP REM L15 (0 DUPLICATES REMOVED)
                      ANSWERS '1-225' FROM FILE HCAPLUS
                      ANSWERS '226-243' FROM FILE USPATFULL
                  D L16 226-243 IBIB HITSTR

     FILE 'REGISTRY' ENTERED AT 14:35:10 ON 31 AUG 2005
L17               STRUCTURE UPLOADED
L18            359 SEA SUB=L9 SSS FUL L17
L19               STRUCTURE UPLOADED
                  D L1
L20           1151 SEA SUB=L3 SSS FUL L19
                  D QUE STA
L21           1151 SEA SUB=L20 SSS FUL L4
L22               STRUCTURE UPLOADED
L23            232 SEA SUB=L20 SSS FUL L22

     FILE 'HCAPLUS, USPATFULL' ENTERED AT 14:42:34 ON 31 AUG 2005
L24           136 SEA PLU=ON  L23
L25           113 SEA PLU=ON  L24 AND (PD<20030129 OR PRD<20030129)
L26           108 DUP REM L25 (5 DUPLICATES REMOVED)
                      ANSWERS '1-81' FROM FILE HCAPLUS
                      ANSWERS '82-108' FROM FILE USPATFULL

     FILE 'REGISTRY' ENTERED AT 14:44:13 ON 31 AUG 2005
L27               STRUCTURE UPLOADED
L28            43 SEA SUB=L23 SSS FUL L27
                  D QUE STA

     FILE 'HCAPLUS, USPATFULL' ENTERED AT 14:45:45 ON 31 AUG 2005
L29            15 SEA PLU=ON  L28
L30            14 SEA PLU=ON  L28 AND (PD<20030129 OR PRD<20030129)
L31            13 DUP REM L30 (1 DUPLICATE REMOVED)
                      ANSWERS '1-9' FROM FILE HCAPLUS
                      ANSWERS '10-13' FROM FILE USPATFULL
L32            13 SEA PLU=ON  L31 AND L26
                  D QUE STA
                  D L32 1-13 IBIB HITSTR
```

FILE HOME

FILE REGISTRY
Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 AUG 2005 HIGHEST RN 862155-39-3
DICTIONARY FILE UPDATES: 30 AUG 2005 HIGHEST RN 862155-39-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
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* available and contains the CA role and document type information. *
* *
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

FILE HCAPLUS
FILE COVERS 1907 - 31 Aug 2005 VOL 143 ISS 10
FILE LAST UPDATED: 30 Aug 2005 (20050830/ED)

FILE USPATFULL
FILE COVERS 1971 TO PATENT PUBLICATION DATE: 30 Aug 2005 (20050830/PD)
FILE LAST UPDATED: 30 Aug 2005 (20050830/ED)
CA INDEXING IS CURRENT THROUGH 30 Aug 2005 (20050830/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 30 Aug 2005 (20050830/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2005

FILE TOXCENTER
FILE COVERS 1907 TO 30 Aug 2005 (20050830/ED)

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=> d his ful

     (FILE 'REGISTRY' ENTERED AT 15:38:28 ON 31 AUG 2005)
                DEL HIS
L1              STRUCTURE UPLOADED
L2              STRUCTURE UPLOADED
L3          2305 SEA SSS FUL L2
L4             0 SEA SUB=L3 SSS FUL L1
L5              STRUCTURE UPLOADED
L6             0 SEA SSS FUL L5
L7              STRUCTURE UPLOADED
L8             2 SEA SSS SAM L7
L9            30 SEA SSS FUL L7

     FILE 'HCAPLUS, USPATFULL' ENTERED AT 15:48:07 ON 31 AUG 2005
L10            5 SEA PLU=ON  L9
L11            5 DUP REM L10 (0 DUPLICATES REMOVED)
                       ANSWERS '1-3' FROM FILE HCAPLUS
                       ANSWERS '4-5' FROM FILE USPATFULL
                 D L11 1-5 IBIB HITSTR

     FILE 'MARPAT' ENTERED AT 15:49:26 ON 31 AUG 2005

     FILE 'REGISTRY' ENTERED AT 15:58:38 ON 31 AUG 2005
L12             STRUCTURE UPLOADED
L13           10 SEA SSS FUL L12

     FILE 'HCAPLUS, USPATFULL' ENTERED AT 15:59:29 ON 31 AUG 2005
L14            4 SEA PLU=ON  L13
L*** DEL       4 DUP REM L14 (0 DUPLICATES REMOVED)
                       ANSWERS '1-2' FROM FILE HCAPLUS
                       ANSWERS '3-4' FROM FILE USPATFULL
                 D L14 1-4 IBIB HITSTR
L15              STRUCTURE UPLOADED

     FILE 'REGISTRY' ENTERED AT 16:04:53 ON 31 AUG 2005
L16           34 SEA SSS FUL L15

     FILE 'HCAPLUS' ENTERED AT 16:04:58 ON 31 AUG 2005
L17            5 SEA PLU=ON  L16
                 D L17 1-5 CBIB
                 D L17 1-5 IBIB HITSTR

     FILE 'REGISTRY' ENTERED AT 16:13:56 ON 31 AUG 2005
L18              STRUCTURE UPLOADED
L19              STRUCTURE UPLOADED
L20              STRUCTURE UPLOADED
L21              STRUCTURE UPLOADED
L22            6 SEA SSS FUL L18
L23           10 SEA SSS FUL L19
L24            2 SEA SSS FUL L20
L25            0 SEA SSS FUL L21
L*** DEL      18 L22 OR L23 OR L24

     FILE 'HCAPLUS' ENTERED AT 16:18:30 ON 31 AUG 2005
L26           10 SEA PLU=ON  L22 OR L23 OR L24
L27           10 DUP REM L26 (0 DUPLICATES REMOVED)
                       ANSWERS '1-10' FROM FILE HCAPLUS
L28           10 SEA L27
L29            3 SEA L11
L30           10 SEA PLU=ON  L28 NOT L29 OR L14
                 D L30 1-10 IBIB HITSTR

     FILE 'STNGUIDE' ENTERED AT 16:22:17 ON 31 AUG 2005
```

```
     FILE 'CASREACT' ENTERED AT 16:23:20 ON 31 AUG 2005
L31            0 SEA PLU=ON  L22
L32            0 SEA SSS SAM L18 (     0 REACTIONS)
L33            0 SEA SSS FUL L18 (     0 REACTIONS)
L34            0 SEA SSS FUL L19 (     0 REACTIONS)
L35            1 SEA SSS FUL L20 (     1 REACTIONS)
                 D L35 CBIB
L36            0 SEA PLU=ON  L23
                 D L35 HITRXN
L37            0 SEA SSS FUL L15 (     0 REACTIONS)
L38            0 SEA SSS FUL L12 (     0 REACTIONS)


     FILE HCAPLUS
     FILE COVERS 1907 - 31 Aug 2005  VOL 143 ISS 10
     FILE LAST UPDATED: 30 Aug 2005  (20050830/ED)

     FILE USPATFULL
     FILE COVERS 1971 TO PATENT PUBLICATION DATE: 30 Aug 2005 (20050830/PD)
     FILE LAST UPDATED: 30 Aug 2005 (20050830/ED)
     CA INDEXING IS CURRENT THROUGH 30 Aug 2005 (20050830/UPCA)
     ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 30 Aug 2005 (20050830/PD)
     REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2005

     FILE MARPAT
     FILE CONTENT: 1988-PRESENT (VOL 143 ISS 09)(20050826/ED)

     MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
     (COVERAGE TO THESE DATES IS NOT COMPLETE):

     US    6903214 07 JUN 2005
     DE   10350965 25 MAY 2005
     EP    1538192 08 JUN 2005
     JP 2005136379 26 MAY 2005
     WO 2005060437 07 JUL 2005

     Expanded G-group definition display now available.

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   30 AUG 2005  HIGHEST RN 862155-39-3
     DICTIONARY FILE UPDATES:  30 AUG 2005  HIGHEST RN 862155-39-3

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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     ************************************************************
     *                                                          *
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     * available and contains the CA role and document type information. *
     *                                                          *
     ************************************************************
```

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Aug 26, 2005 (20050826/UP).

FILE CASREACT

FILE CONTENT:1840 - 28 Aug 2005 VOL 143 ISS 9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*
* CASREACT now has more than 9.2 million reactions *
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
> d his ful

     (FILE 'HOME' ENTERED AT 17:20:35 ON 31 AUG 2005)

     FILE 'REGISTRY' ENTERED AT 17:20:39 ON 31 AUG 2005
L1                STRUCTURE UPLOADED
L2             17 SEA SSS FUL L1
                  D L2 1-17 ED

     FILE 'HCAPLUS' ENTERED AT 17:21:29 ON 31 AUG 2005
L3              3 SEA PLU=ON  L2
                  D L3 1-3 IBIB

     FILE 'REGISTRY' ENTERED AT 17:46:40 ON 31 AUG 2005
L4                STRUCTURE UPLOADED
L5             20 SEA SSS FUL L4

     FILE 'HCAPLUS' ENTERED AT 17:47:06 ON 31 AUG 2005
L6              1 SEA PLU=ON  L5
                  D L6
L7                STRUCTURE UPLOADED
                  D L7
                  S L7

     FILE 'REGISTRY' ENTERED AT 18:34:56 ON 31 AUG 2005
L8              3 SEA SSS SAM L7

     FILE 'HCAPLUS' ENTERED AT 18:34:57 ON 31 AUG 2005
L9              4 SEA PLU=ON  L8
                  D L9

     FILE 'CASREACT' ENTERED AT 18:35:15 ON 31 AUG 2005
L10             0 SEA SSS SAM L7 (     0 REACTIONS)
L11           105 SEA SSS FUL L7 (   920 REACTIONS)

     FILE 'REGISTRY' ENTERED AT 18:36:57 ON 31 AUG 2005
                  D L8
                  D L8 2-3
L12               STRUCTURE UPLOADED
L13          1922 SEA SSS FUL L12
L14               STRUCTURE UPLOADED
L15            13 SEA SUB=L13 SSS FUL L14

     FILE 'HCAPLUS' ENTERED AT 18:44:43 ON 31 AUG 2005
L16             6 SEA PLU=ON  L15

     FILE 'CASREACT' ENTERED AT 18:45:00 ON 31 AUG 2005
L17             0 SEA PLU=ON  L15
L18             0 SEA SSS SAM L14 (     0 REACTIONS)
L19             0 SEA SSS FUL L14 (     0 REACTIONS)

     FILE 'HCAPLUS' ENTERED AT 18:45:34 ON 31 AUG 2005
                  D L16 1-6 IBIB HITSTR

     FILE 'STNGUIDE' ENTERED AT 18:47:07 ON 31 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 18:49:08 ON 31 AUG 2005
                  SET LINE 250
                  SET DETAIL OFF
                  E "146474-01-3"/BI,RN 25
                  SET NOTICE 1000 SEARCH
L20             2 SEA PLU=ON  146474-01-3/BI
L21             2 SEA PLU=ON  146474-01-3/BI
                  SET NOTICE OFF DISPLAY
```

```
                SET LINE LOGIN
                SET DETAIL LOGIN
                DIS L21 1 HIT
                DIS L21 2 HIT
                DIS L21 1 IBIB
                DIS L21 2 IBIB
                SET NOTICE LOGIN DISPLAY
                SET NOTICE LOGIN SEARCH

     FILE 'REGISTRY' ENTERED AT 18:55:05 ON 31 AUG 2005
L22             STRUCTURE UPLOADED
L23          248 SEA SUB=L13 SSS FUL L22

     FILE 'HCAPLUS' ENTERED AT 18:56:00 ON 31 AUG 2005
L24          180 SEA PLU=ON  L23
L25          138 SEA PLU=ON  L24 AND PD<20030129
L26           80 SEA PLU=ON  L24 AND PRD<20030129
L27          122 SEA PLU=ON  L24 AND PD<20020129
                D L27 1-5 IBIB HITSTR

     FILE 'STNGUIDE' ENTERED AT 18:58:14 ON 31 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 19:00:41 ON 31 AUG 2005

     FILE 'STNGUIDE' ENTERED AT 19:05:31 ON 31 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 19:09:34 ON 31 AUG 2005
                D L27 110-122 IBIB HITSTR

     FILE 'STNGUIDE' ENTERED AT 19:09:36 ON 31 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 19:16:25 ON 31 AUG 2005
                D L27 100-109 IBIB HITSTR

     FILE 'STNGUIDE' ENTERED AT 19:16:28 ON 31 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 19:17:26 ON 31 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 19:17:27 ON 31 AUG 2005
L28           13 SEA PLU=ON  L27 AND FLUORO?
                D L28 1-13 IBIB HITSTR KWIC

     FILE 'STNGUIDE' ENTERED AT 19:18:27 ON 31 AUG 2005


     FILE HOME

     FILE REGISTRY
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     DICTIONARY FILE UPDATES:  30 AUG 2005  HIGHEST RN 862155-39-3

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     *                                                          *
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```
* the IDE default display format and the ED field has been added,    *
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*                                                                    *
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FILE HCAPLUS

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FILE COVERS 1907 - 31 Aug 2005  VOL 143 ISS 10
FILE LAST UPDATED: 30 Aug 2005  (20050830/ED)

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FILE CASREACT
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FILE CONTENT:1840 - 28 Aug 2005 VOL 143 ISS 9

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identification.

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Aug 26, 2005 (20050826/UP).

=> d que sta
L12             STR
```
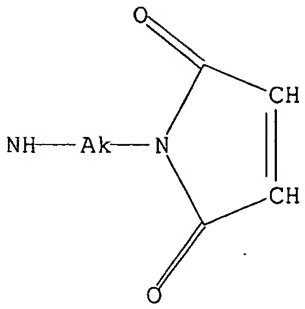
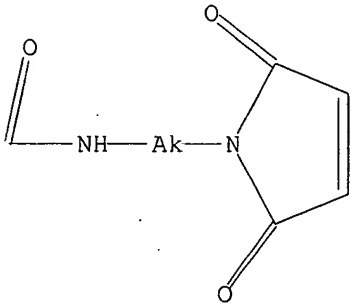
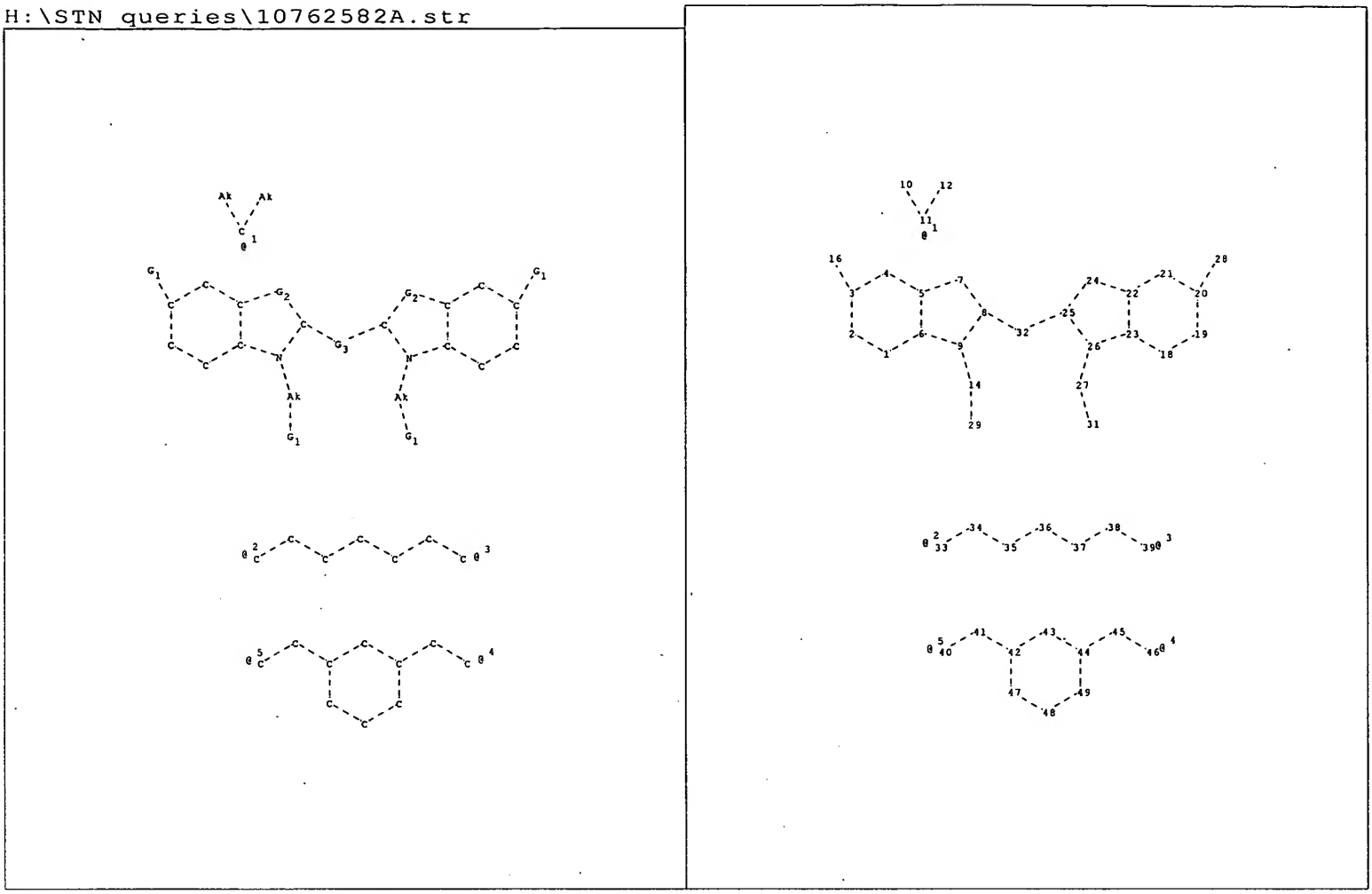



Structure attributes must be viewed using STN Express query preparation.
L13 1922 SEA FILE=REGISTRY SSS FUL L12
L22 STR



Structure attributes must be viewed using STN Express query preparation.
L23 248 SEA FILE=REGISTRY SUB=L13 SSS FUL L22
L24 180 SEA FILE=HCAPLUS PLU=ON L23
L27 122 SEA FILE=HCAPLUS PLU=ON L24 AND PD<20020129
L28 13 SEA FILE=HCAPLUS PLU=ON L27 AND FLUORO?

H:\STN queries\10762582A.str



chain nodes :
10 11 12 14 16 27 28 29 31 32 33 34 35 36 37 38 39 40 41
45 46
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26 42 43 44
47 48 49
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-32 26-27 27-31 33-34
34-35 35-36 36-37 37-38 38-39 40-41 41-42 44-45 45-46
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26 42-43 42-47 43-44 44-49
47-48 48-49
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-32 26-27 27-31 33-34 34-35 35-36 36-37 37-38 38-39
40-41 41-42 42-43 42-47 43-44 44-45 44-49 45-46 47-48 48-49

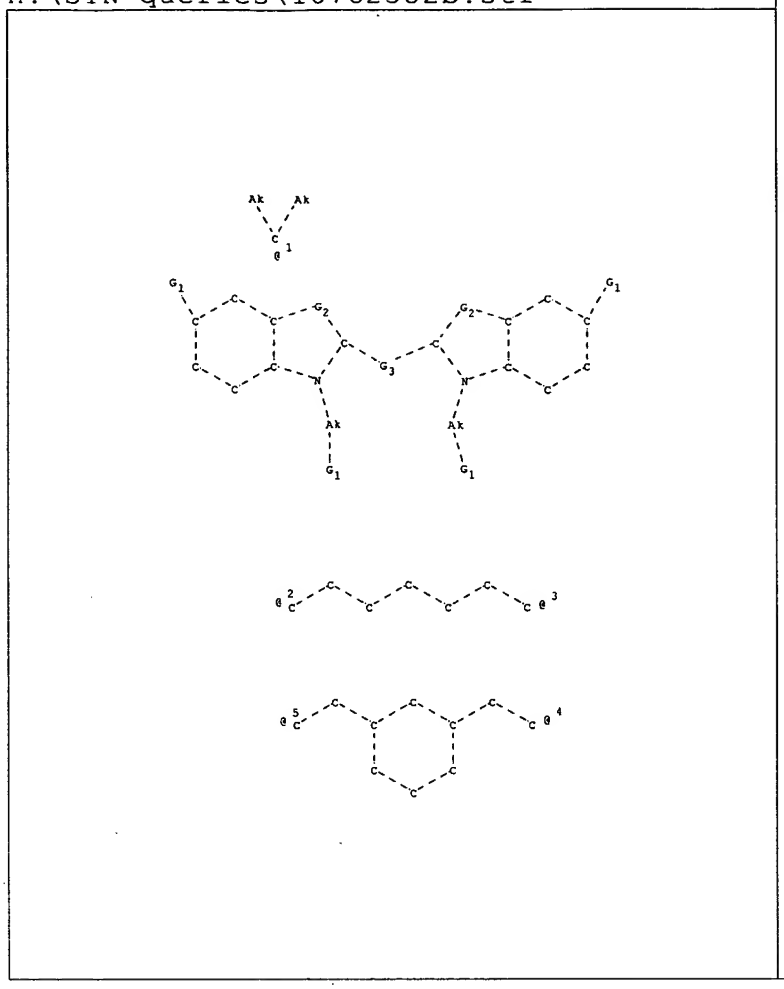
G1:H,SO3H

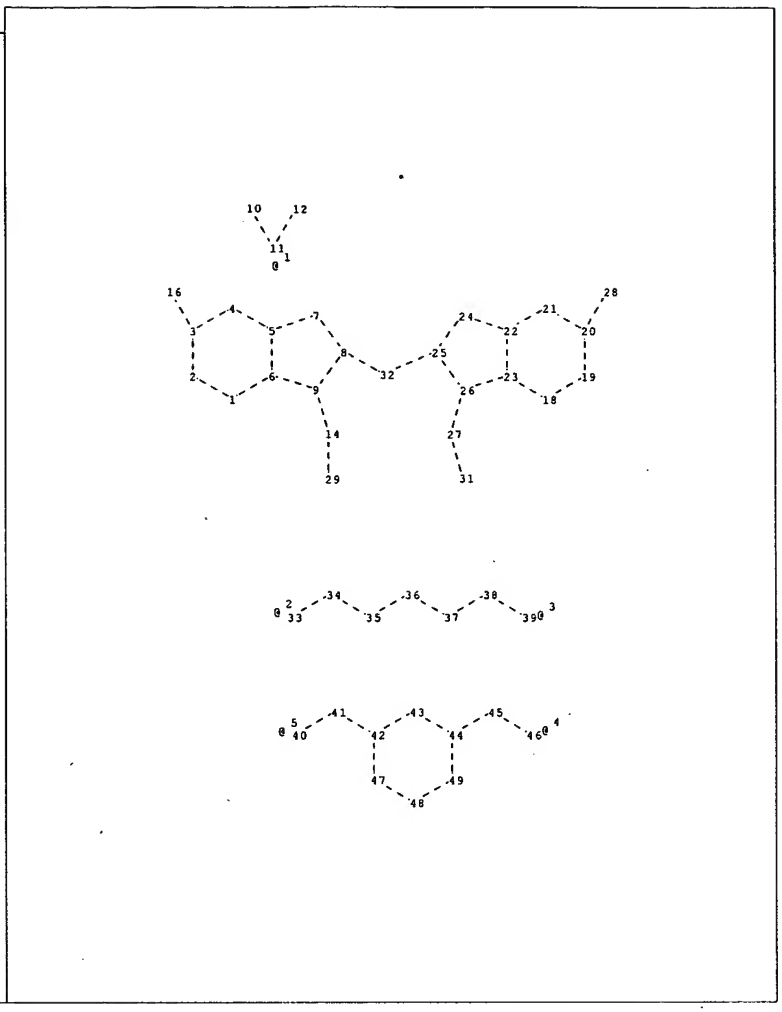
G2:O,S,[*1]

G3:[*2-*3],[*4-*5]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
29:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:Atom 43:Atom 44:Atom
45:CLASS 46:CLASS 47:Atom 48:Atom 49:Atom

H:\STN queries\10762582b.str





chain nodes :
10 11 12 14 16 27 28 29 31 32 33 34 35 36 37 38 39 40 41
45 46
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26 42 43 44
47 48 49
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-32 26-27 27-31 33-34
34-35 35-36 36-37 37-38 38-39 40-41 41-42 44-45 45-46
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26 42-43 42-47 43-44 44-49
47-48 48-49
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-32 26-27 27-31 33-34 34-35 35-36 36-37 37-38 38-39
40-41 41-42 42-43 42-47 43-44 44-45 44-49 45-46 47-48 48-49

G1:H,SO3H

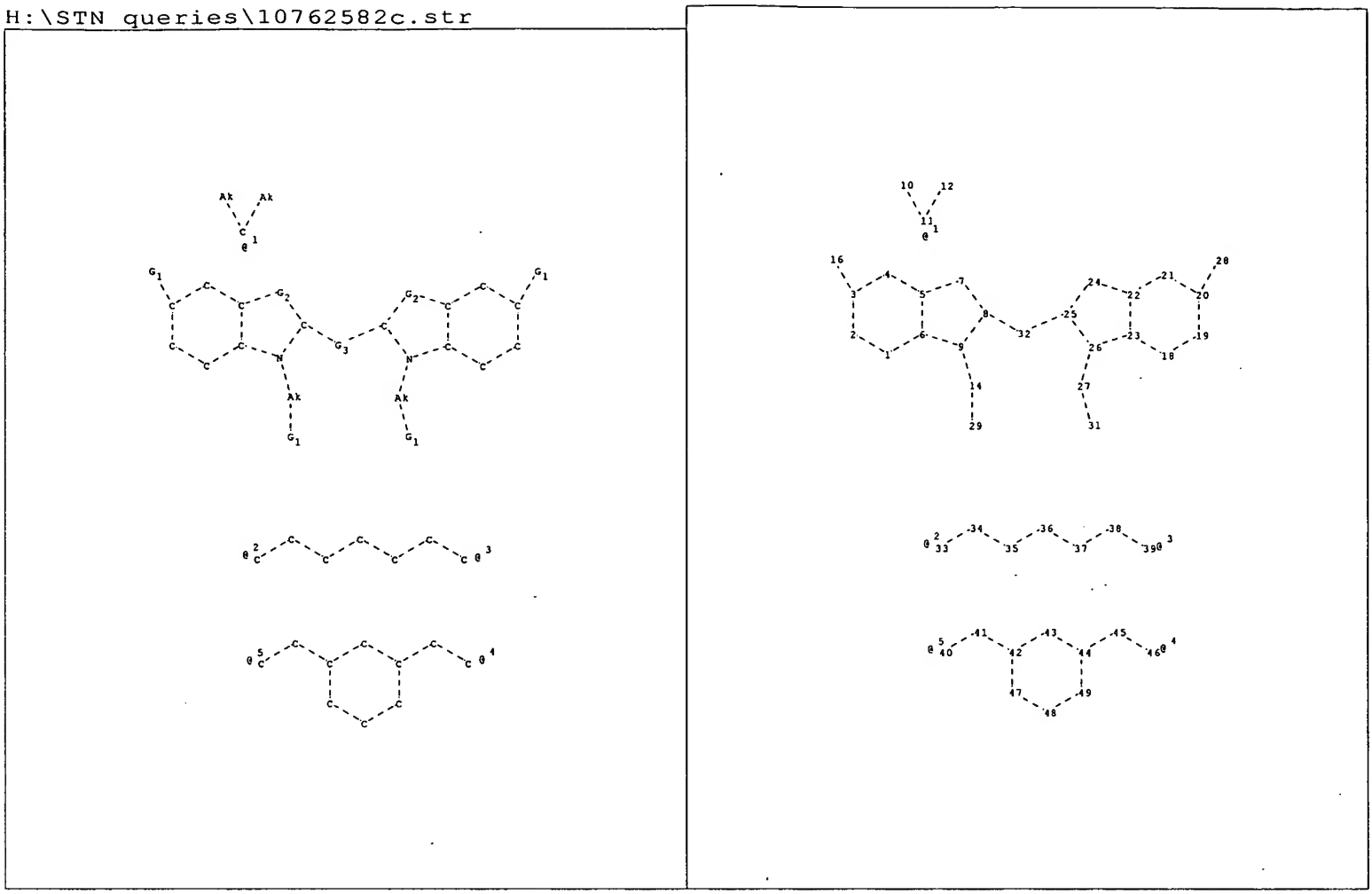
G2:O,S,[*1]

G3:[*2-*3],[*4-*5]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
29:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:Atom 43:Atom 44:Atom
45:CLASS 46:CLASS 47:Atom 48:Atom 49:Atom
Generic attributes :

14:
Type of chain : Linear
Number of Carbon Atoms : less than 7
27:
Type of chain : Linear
Number of Carbon Atoms : less than 7

H:\STN queries\10762582c.str



chain nodes :
10 11 12 14 16 27 28 29 31 32 33 34 35 36 37 38 39 40 41
45 46
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26 42 43 44
47 48 49
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-32 26-27 27-31 33-34
34-35 35-36 36-37 37-38 38-39 40-41 41-42 44-45 45-46
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26 42-43 42-47 43-44 44-49
47-48 48-49
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-32 26-27 27-31 33-34 34-35 35-36 36-37 37-38 38-39
40-41 41-42 42-43 42-47 43-44 44-45 44-49 45-46 47-48 48-49

G1:H,SO3H

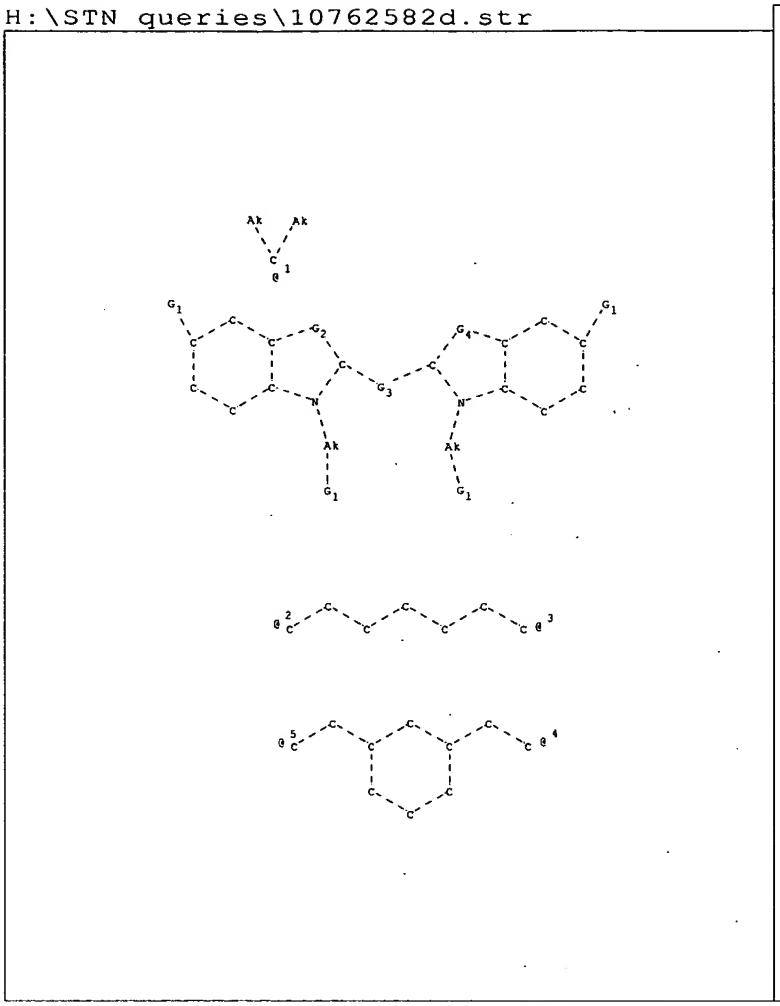
G2:O,S,[*1]

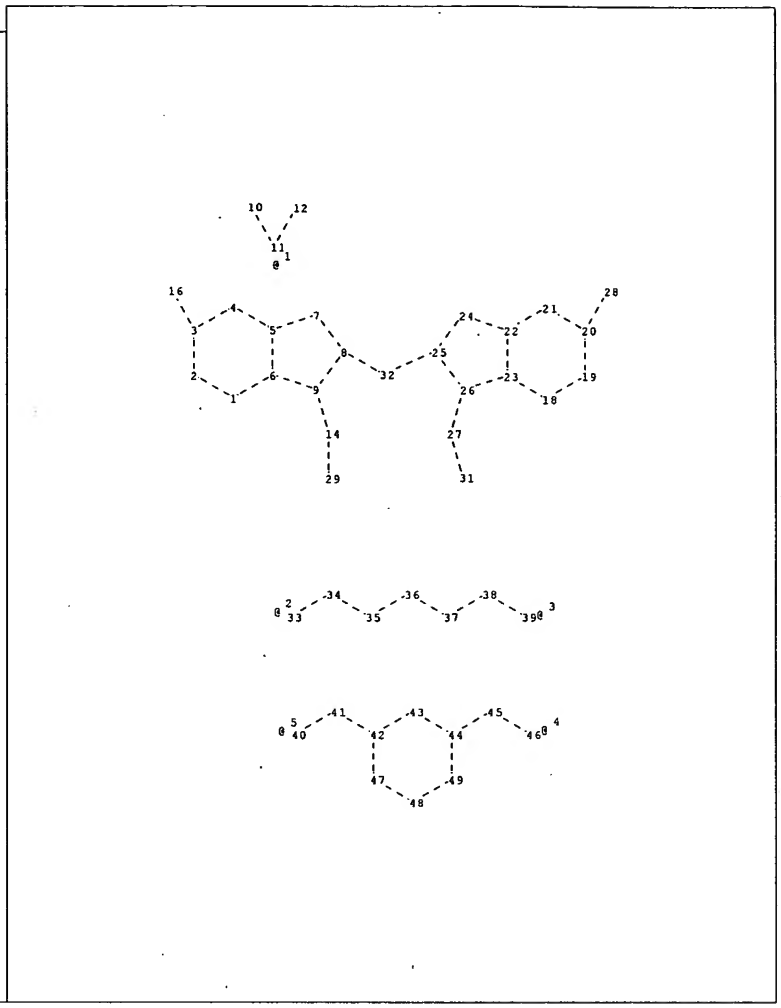
G3:[*2-*3],[*4-*5]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
29:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:Atom 43:Atom 44:Atom
45:CLASS 46:CLASS 47:Atom 48:Atom 49:Atom
Generic attributes :

10:
Type of chain : Linear
Number of Carbon Atoms : less than 7
12:
Type of chain : Linear
Number of Carbon Atoms : less than 7
14:
Type of chain : Linear
Number of Carbon Atoms : less than 7
27:
Type of chain : Linear
Number of Carbon Atoms : less than 7

H:\STN queries\10762582d.str





chain nodes :
10 11 12 14 16 27 28 29 31 32 33 34 35 36 37 38 39 40 41
45 46
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26 42 43 44
47 48 49
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-32 26-27 27-31 33-34
34-35 35-36 36-37 37-38 38-39 40-41 41-42 44-45 45-46
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26 42-43 42-47 43-44 44-49
47-48 48-49
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-32 26-27 27-31 33-34 34-35 35-36 36-37 37-38 38-39
40-41 41-42 42-43 42-47 43-44 44-45 44-49 45-46 47-48 48-49

G1:H,SO3H

G2:O,S,[*1]

G3:[*2-*3],[*4-*5]

G4:S,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
29:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:Atom 43:Atom 44:Atom
45:CLASS

46:CLASS 47:Atom 48:Atom 49:Atom

Generic attributes :

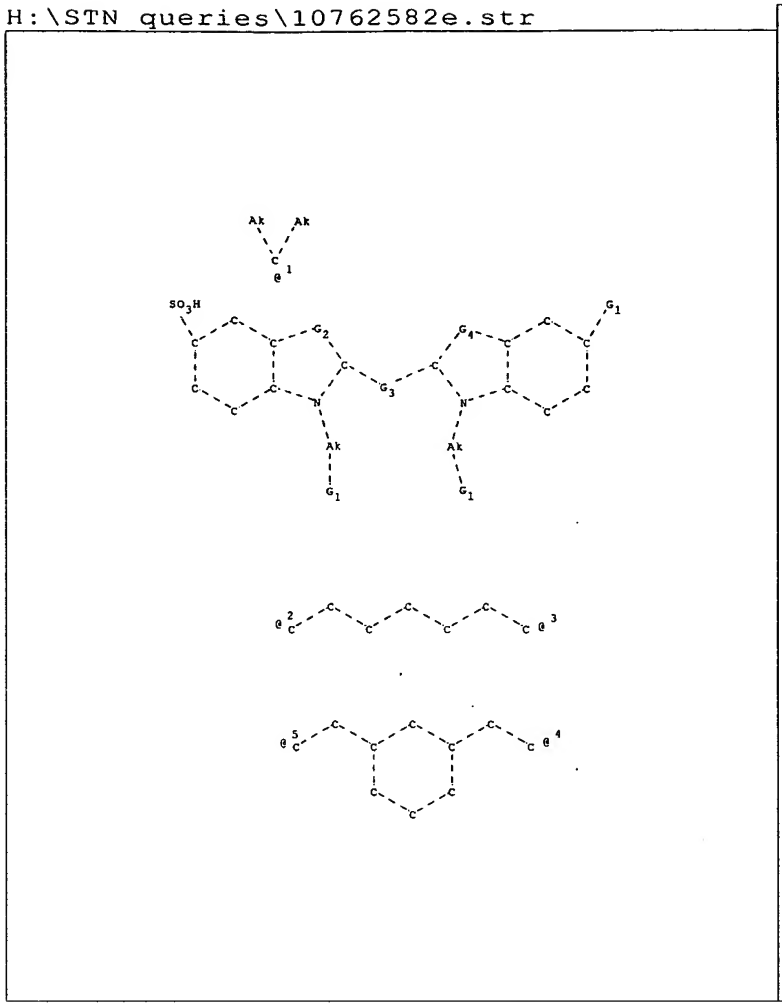
10:
Type of chain : Linear
Number of Carbon Atoms : less than 7

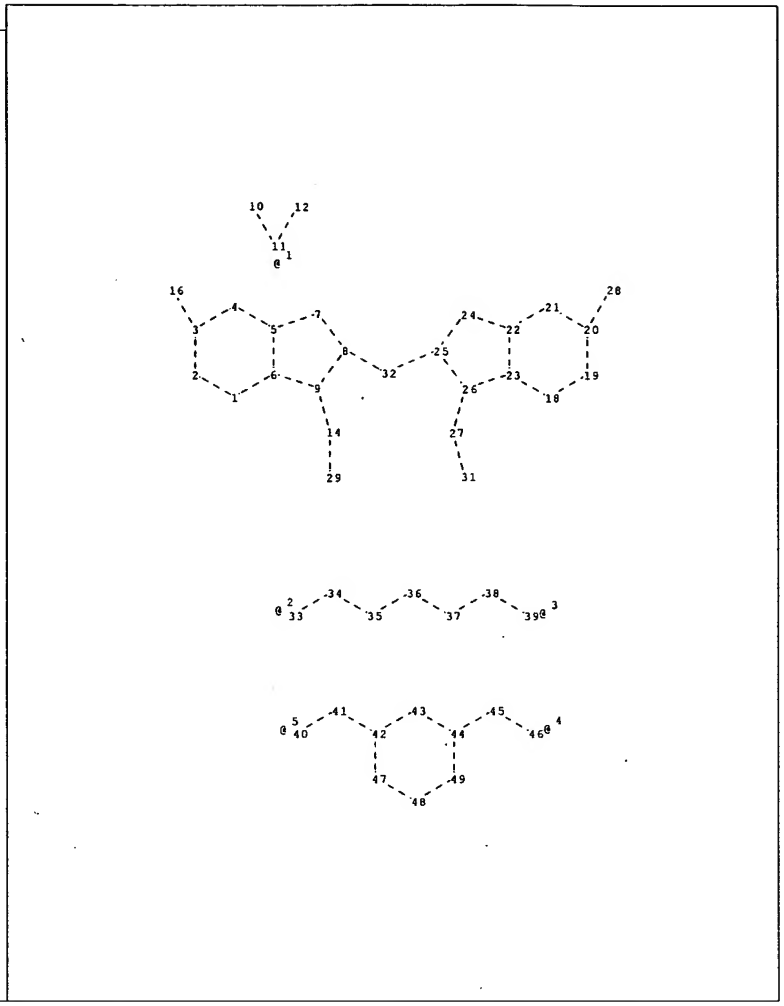
12:
Type of chain : Linear
Number of Carbon Atoms : less than 7

14:
Type of chain : Linear
Number of Carbon Atoms : less than 7

27:
Type of chain : Linear
Number of Carbon Atoms : less than 7

H:\STN queries\10762582e.str





chain nodes :
10 11 12 14 16 27 28 29 31 32 33 34 35 36 37 38 39 40 41
45 46
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26 42 43 44
47 48 49
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-32 26-27 27-31 33-34
34-35 35-36 36-37 37-38 38-39 40-41 41-42 44-45 45-46
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26 42-43 42-47 43-44 44-49
47-48 48-49
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-32 26-27 27-31 33-34 34-35 35-36 36-37 37-38 38-39
40-41 41-42 42-43 42-47 43-44 44-45 44-49 45-46 47-48 48-49

G1:H,SO3H

G2:O,S,[*1]

G3:[*2-*3],[*4-*5]

G4:S,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
29:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:Atom 43:Atom 44:Atom
45:CLASS

46:CLASS 47:Atom 48:Atom 49:Atom

Generic attributes :

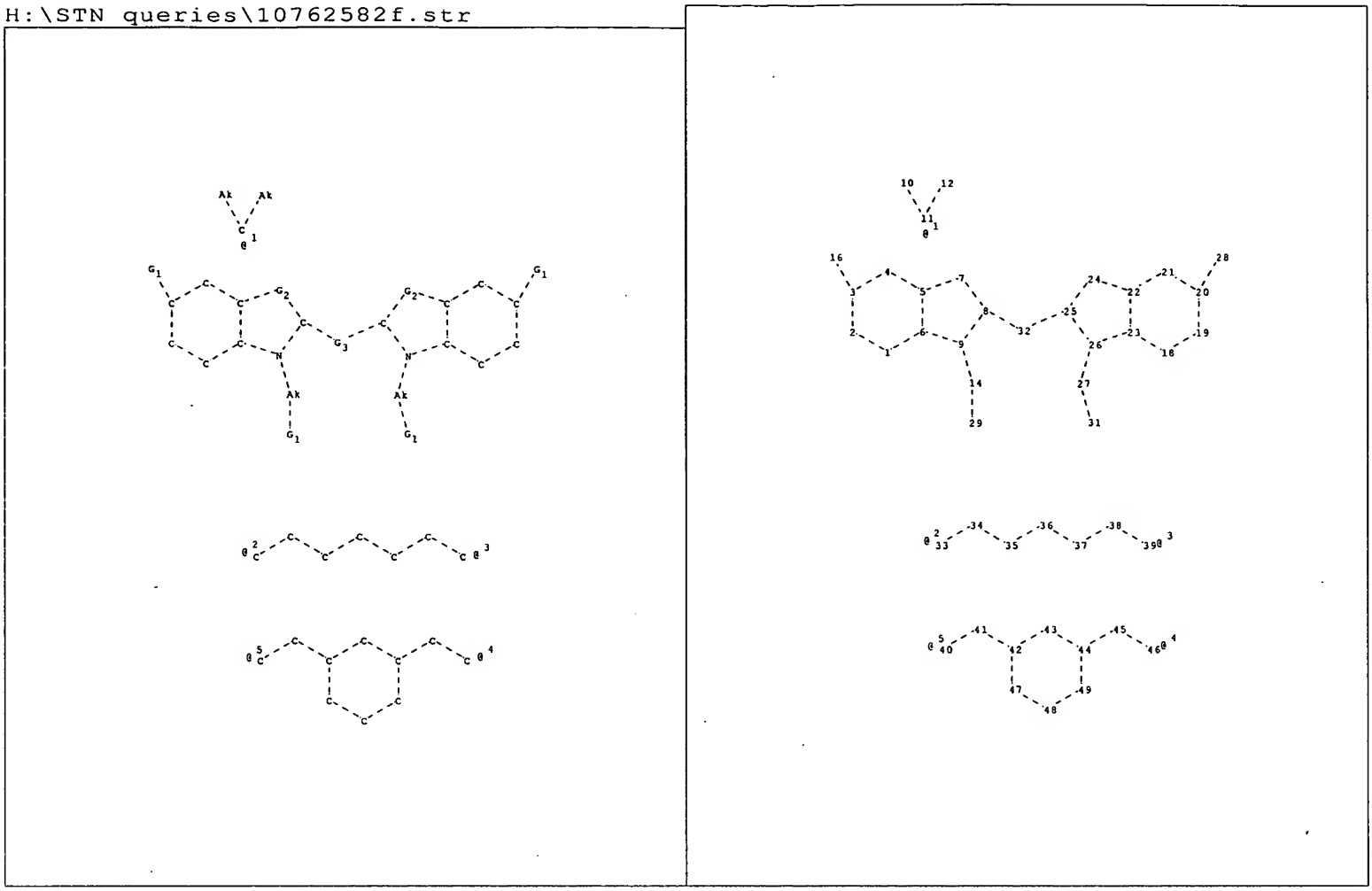
10:
Type of chain : Linear
Number of Carbon Atoms : less than 7

12:
Type of chain : Linear
Number of Carbon Atoms : less than 7

14:
Type of chain : Linear
Number of Carbon Atoms : less than 7

27:
Type of chain : Linear
Number of Carbon Atoms : less than 7

H:\STN queries\10762582f.str



chain nodes :
10 11 12 14 16 27 28 29 31 32 33 34 35 36 37 38 39 40 41
45 46
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26 42 43 44
47 48 49
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-32 26-27 27-31 33-34
34-35 35-36 36-37 37-38 38-39 40-41 41-42 44-45 45-46
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26 42-43 42-47 43-44 44-49
47-48 48-49
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-32 26-27 27-31 33-34 34-35 35-36 36-37 37-38 38-39
40-41 41-42 42-43 42-47 43-44 44-45 44-49 45-46 47-48 48-49

G1:H,SO3H

G2:O,S,[*1]

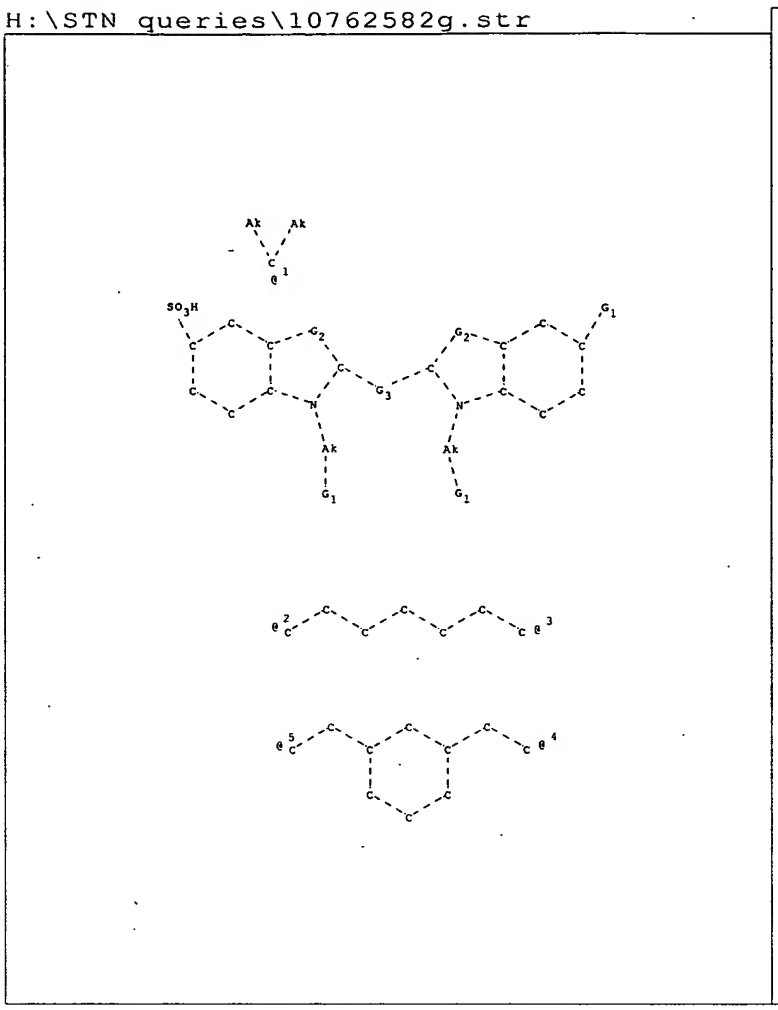
G3:[*2-*3],[*4-*5]

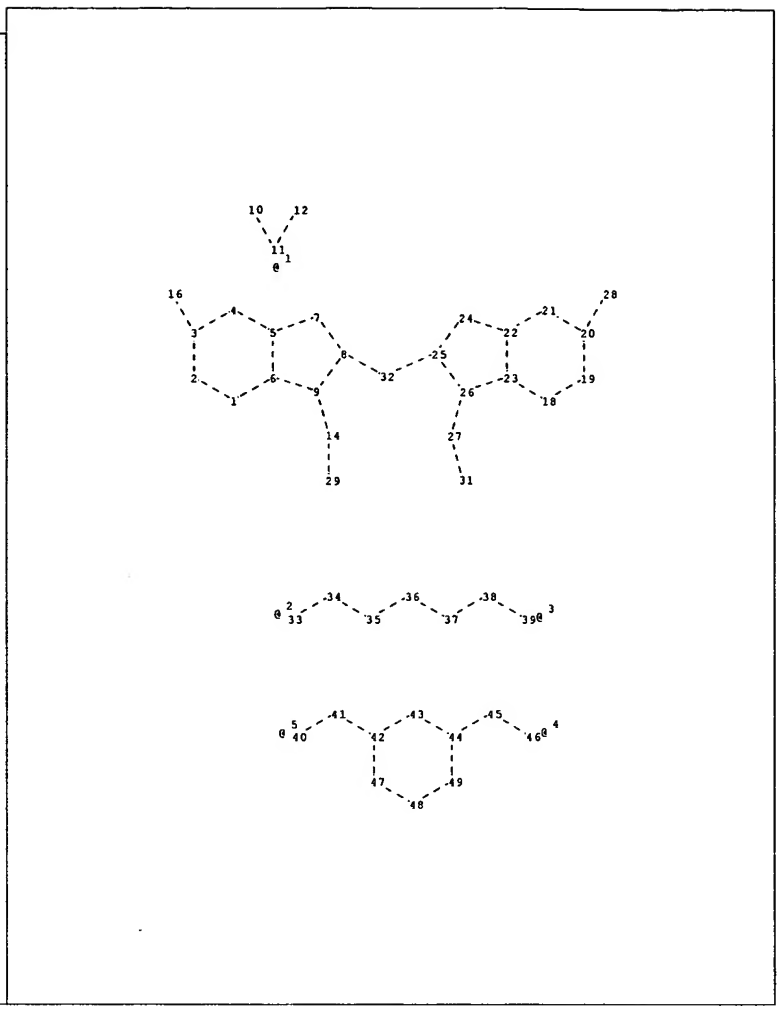
G4:S,[*1]

Hydrogen count :
36:= exact 0 43:= exact 0
Connectivity :
36:3 E exact RC ring/chain 43:3 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS

```
            11:CLASS  12:CLASS  14:CLASS  16:CLASS  18:Atom  19:Atom  20:Atom
    21:Atom  22:Atom  23:Atom  24:Atom  25:Atom  26:Atom  27:CLASS  28:CLASS
    29:CLASS  31:CLASS  32:CLASS  33:CLASS  34:CLASS  35:CLASS  36:CLASS
    37:CLASS  38:CLASS  39:CLASS  40:CLASS  41:CLASS  42:Atom  43:Atom  44:Atom
    45:CLASS  46:CLASS  47:Atom  48:Atom  49:Atom
Generic attributes :
    10:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
    12:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
    14:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
    27:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
```

H:\STN queries\10762582g.str





chain nodes :
10 11 12 14 16 27 28 29 31 32 33 34 35 36 37 38 39 40 41
45 46
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26 42 43 44
47 48 49
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-32 26-27 27-31 33-34
34-35 35-36 36-37 37-38 38-39 40-41 41-42 44-45 45-46
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26 42-43 42-47 43-44 44-49
47-48 48-49
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-32 26-27 27-31 33-34 34-35 35-36 36-37 37-38 38-39
40-41 41-42 42-43 42-47 43-44 44-45 44-49 45-46 47-48 48-49

G1:H,SO3H

G2:O,S,[*1]

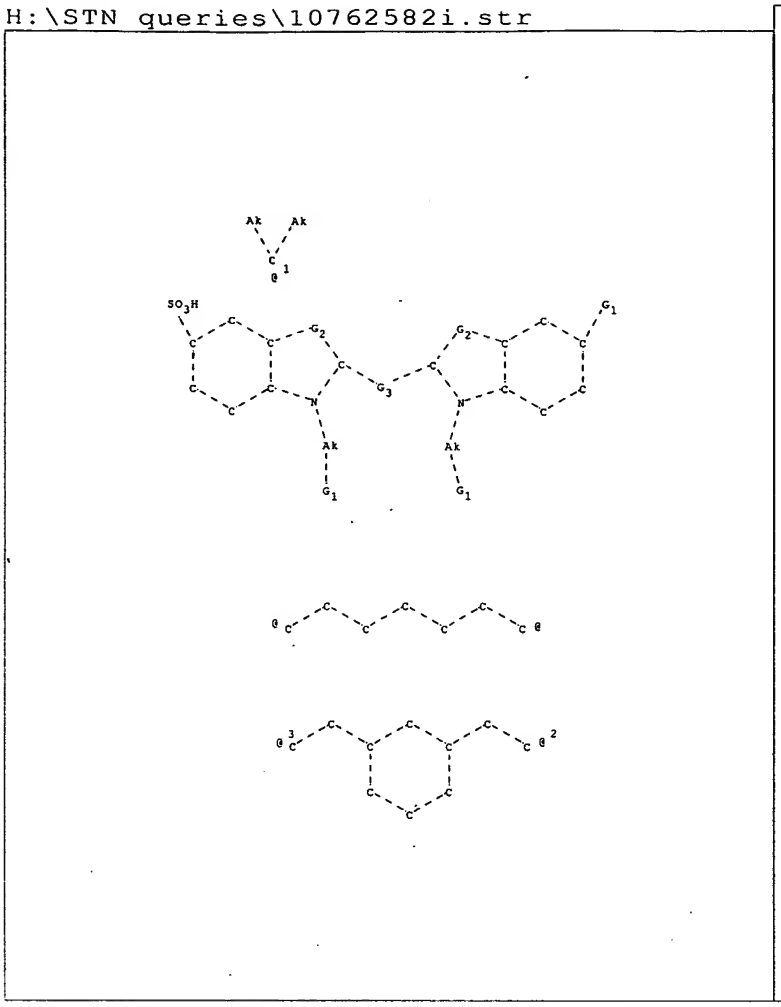
G3:[*2-*3],[*4-*5]

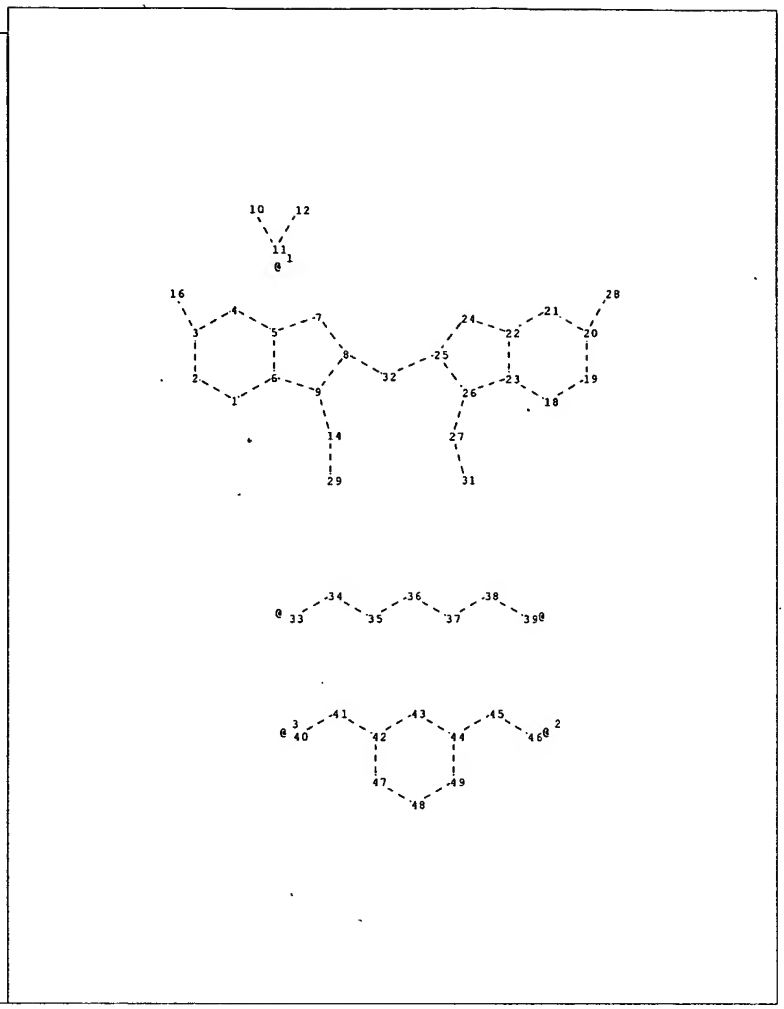
G4:S,[*1]

Hydrogen count :
36:= exact 0 43:= exact 0
Connectivity :
36:3 E exact RC ring/chain 43:3 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS

```
            11:CLASS  12:CLASS  14:CLASS  16:CLASS  18:Atom  19:Atom  20:Atom
    21:Atom  22:Atom  23:Atom  24:Atom  25:Atom  26:Atom  27:CLASS  28:CLASS
    29:CLASS  31:CLASS  32:CLASS  33:CLASS  34:CLASS  35:CLASS  36:CLASS
    37:CLASS  38:CLASS  39:CLASS  40:CLASS  41:CLASS  42:Atom  43:Atom  44:Atom
    45:CLASS  46:CLASS  47:Atom  48:Atom  49:Atom
Generic attributes :
    10:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
    12:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
    14:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
    27:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
```

H:\STN queries\10762582i.str





chain nodes :
10 11 12 14 16 27 28 29 31 32 33 34 35 36 37 38 39 40 41
45 46
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26 42 43 44
47 48 49
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-32 26-27 27-31 33-34
34-35 35-36 36-37 37-38 38-39 40-41 41-42 44-45 45-46
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26 42-43 42-47 43-44 44-49
47-48 48-49
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-32 26-27 27-31 33-34 34-35 35-36 36-37 37-38 38-39
40-41 41-42 42-43 42-47 43-44 44-45 44-49 45-46 47-48 48-49

G1:H,SO3H

G2:O,S,[*1]

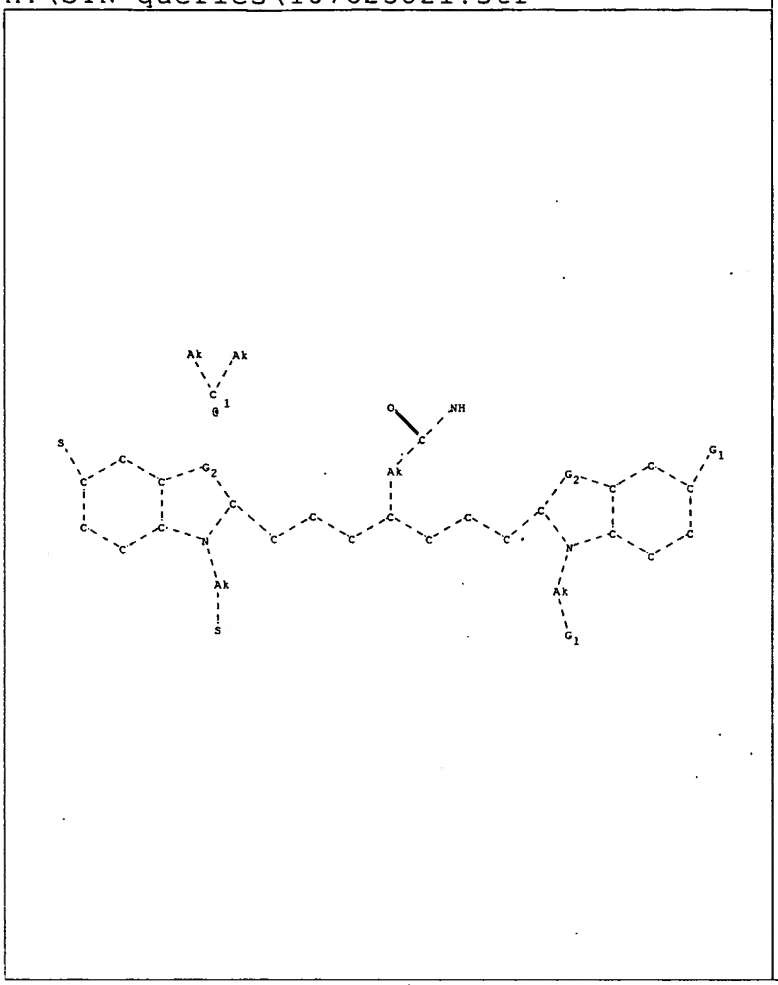
G3:[*2-*3]

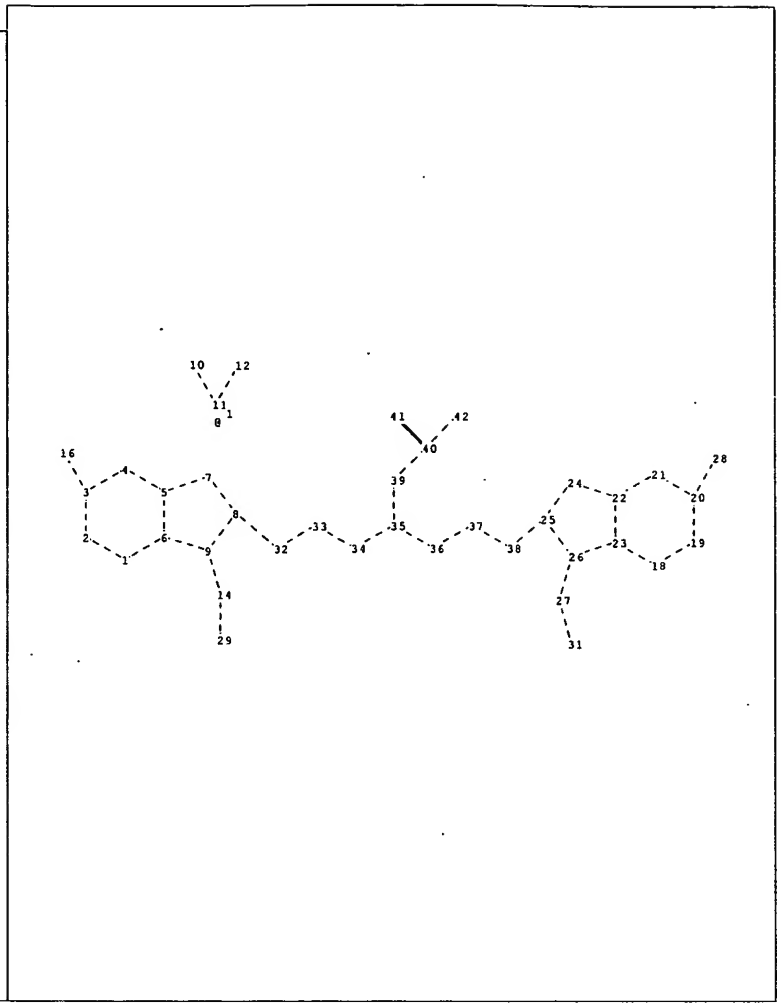
G4:S,[*1]

Hydrogen count :
36:= exact 0 43:= exact 0
Connectivity :
36:3 E exact RC ring/chain 43:3 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS

```
            11:CLASS  12:CLASS  14:CLASS  16:CLASS  18:Atom  19:Atom  20:Atom
    21:Atom  22:Atom  23:Atom  24:Atom  25:Atom  26:Atom  27:CLASS  28:CLASS
    29:CLASS  31:CLASS  32:CLASS  33:CLASS  34:CLASS  35:CLASS  36:CLASS
    37:CLASS  38:CLASS  39:CLASS  40:CLASS  41:CLASS  42:Atom  43:Atom  44:Atom
    45:CLASS  46:CLASS  47:Atom  48:Atom  49:Atom
Generic attributes :
    10:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
    12:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
    14:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
    27:
    Type of chain           : Linear
    Number of Carbon Atoms : less than 7
```

H:\STN queries\10762582l.str





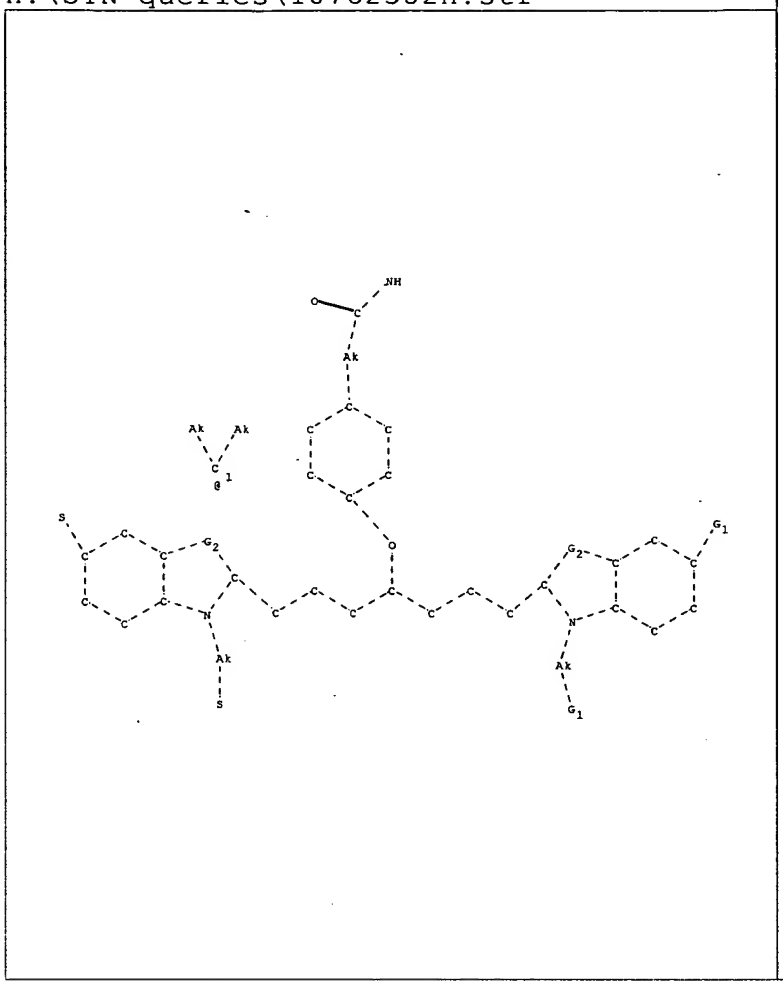
chain nodes :
10 11 12 14 16 27 28 29 31 32 33 37 38 39 40 41 42
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26
ring/chain nodes :
34 35 36
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-38 26-27 27-31 32-33
33-34 35-39 36-37 37-38 39-40 40-41 40-42
ring/chain bonds :
34-35 35-36
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-38 26-27 27-31 32-33 33-34 34-35 35-36 35-39 36-37
37-38 39-40 40-41 40-42

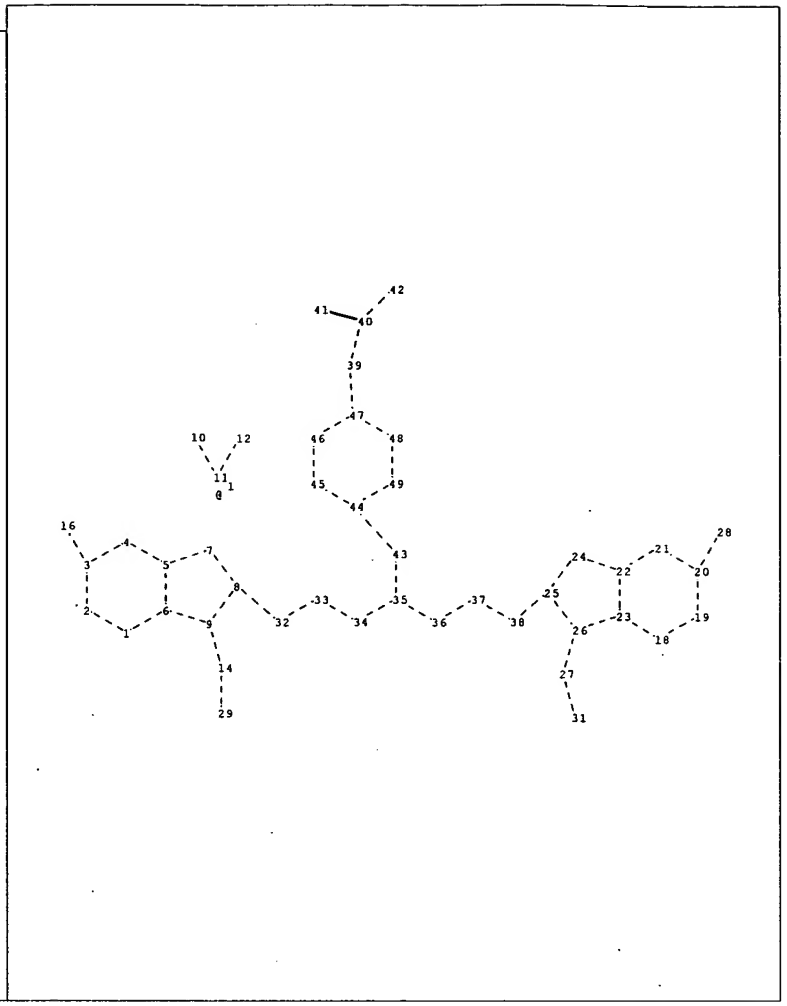
G1:H,SO3H

G2:O,S,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
29:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS

H:\STN queries\10762582n.str





chain nodes :
10 11 12 14 16 27 28 29 31 32 33 37 38 39 40 41 42 43
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26 44 45 46
47 48 49
ring/chain nodes :
34 35 36
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-38 26-27 27-31 32-33
33-34 35-43 36-37 37-38 39-40 39-47 40-41 40-42 43-44
ring/chain bonds :
34-35 35-36
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26 44-45 44-49 45-46 46-47
47-48 48-49
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-38 26-27 27-31 32-33 33-34 34-35 35-36 35-43 36-37
37-38 39-40 39-47 40-41 40-42 43-44 44-45 44-49 45-46 46-47 47-48
48-49

G1:H,SO3H

G2:O,S,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
29:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS
44:Atom

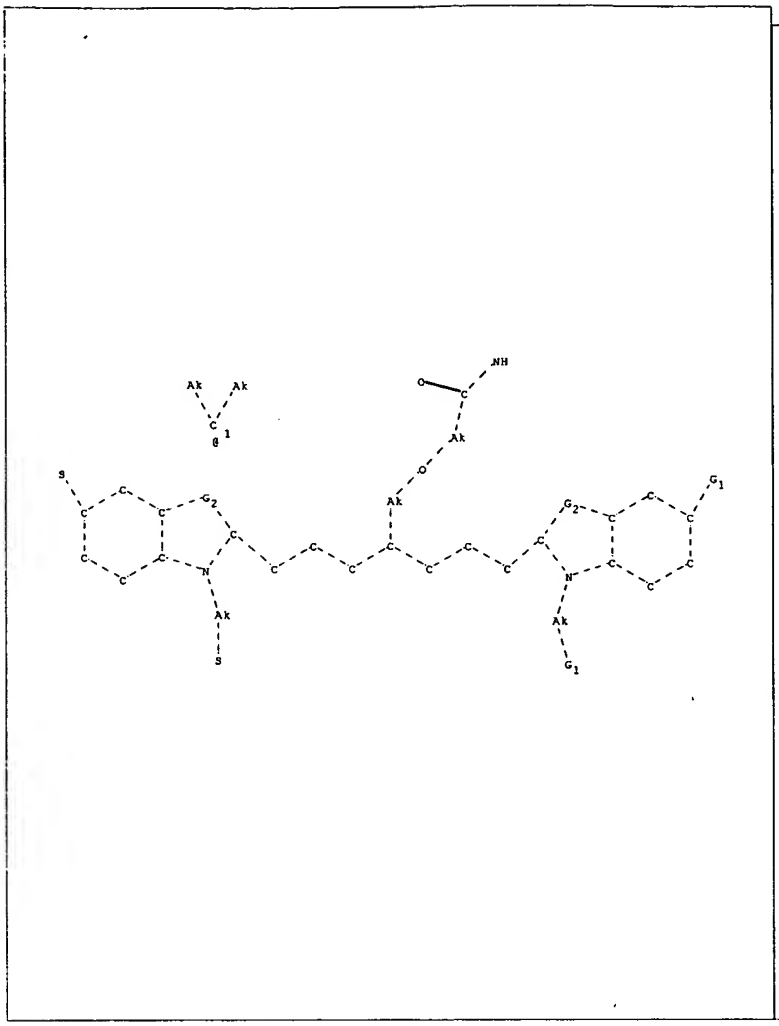
45:Atom 46:Atom 47:Atom 48:Atom 49:Atom

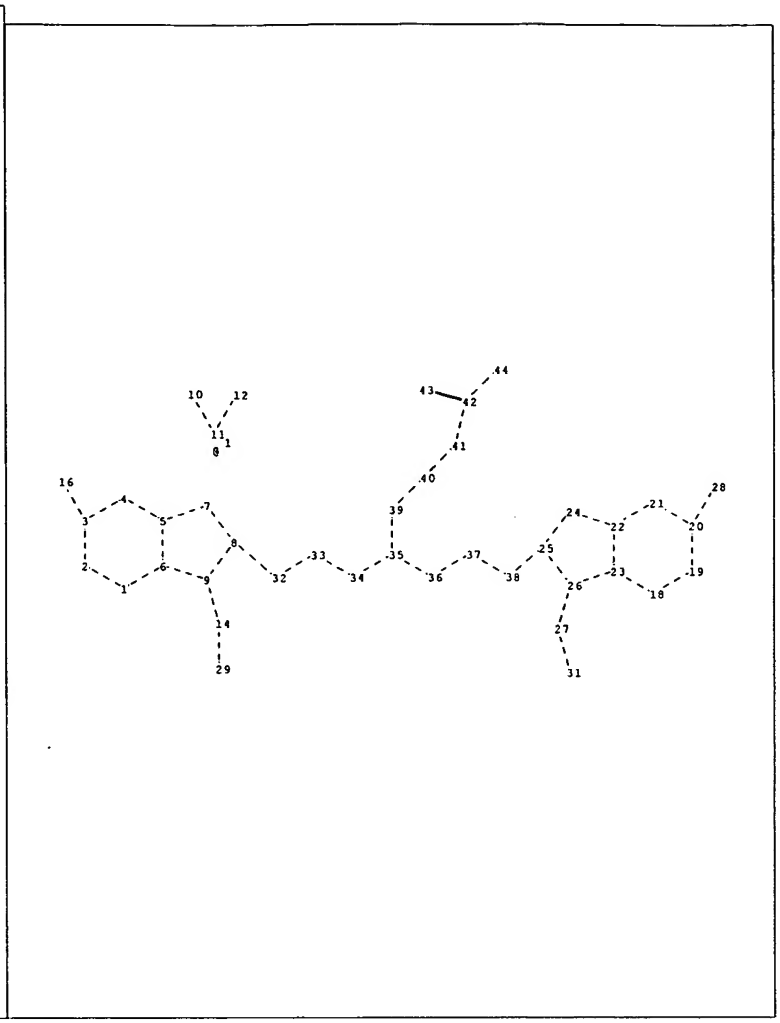
Generic attributes :

39:

Type of chain : Linear

Number of Carbon Atoms : less than 7





chain nodes :
10 11 12 14 16 27 28 29 31 32 33 37 38 39 40 41 42 43 44
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26
ring/chain nodes :
34 35 36
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-38 26-27 27-31 32-33
33-34 35-39 36-37 37-38 39-40 40-41 41-42 42-43 42-44
ring/chain bonds :
34-35 35-36
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-38 26-27 27-31 32-33 33-34 34-35 35-36 35-39 36-37
37-38 39-40 40-41 41-42 42-43 42-44

G1:H,SO3H

G2:O,S,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
29:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS
44:CLASS
Generic attributes :
41:

Type of chain : Linear
Number of Carbon Atoms : less than 7

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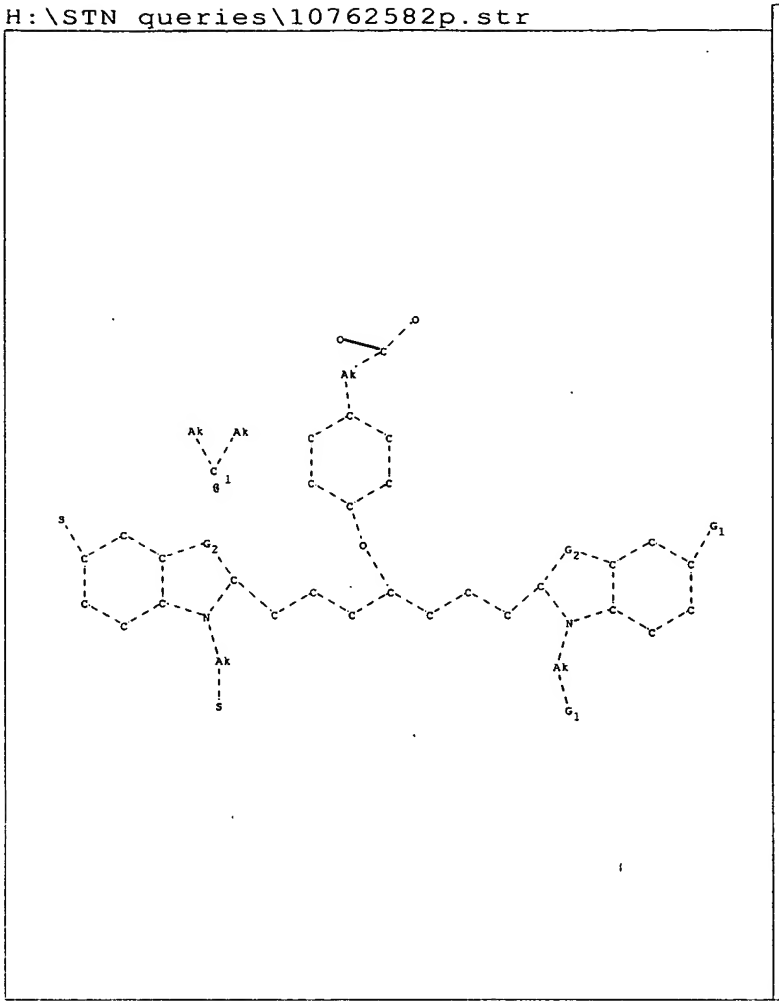

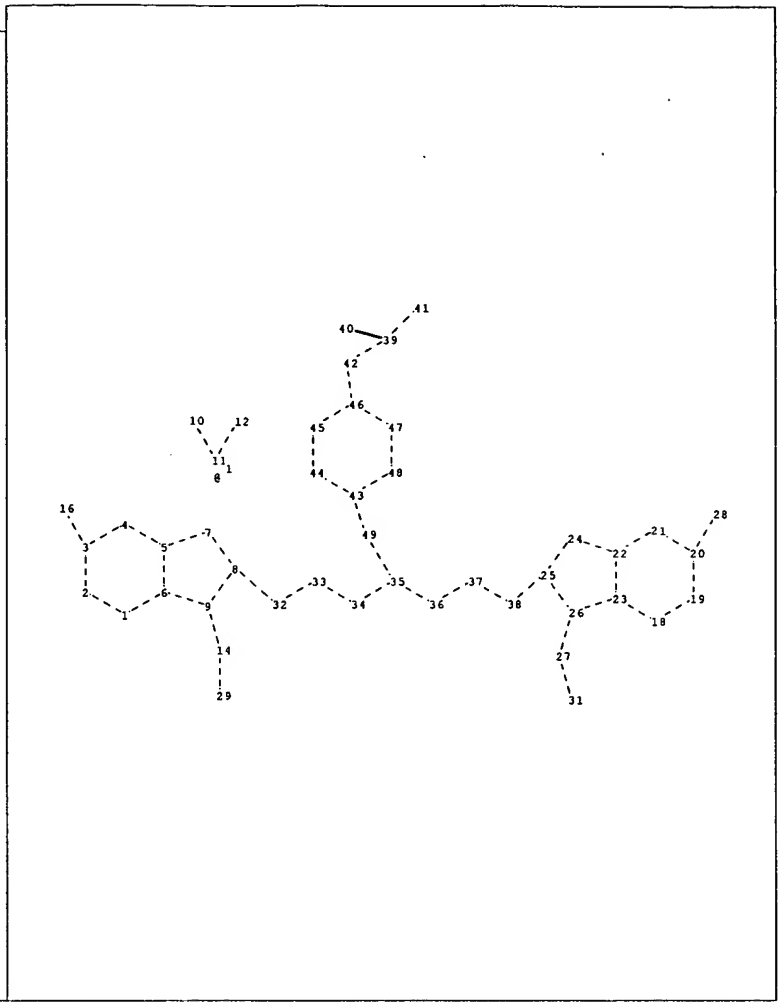

chain nodes :
10 11 12 14 16 27 28 29 31 32 33 37 38 39 40 41 42 49
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26 43 44 45
46 47 48
ring/chain nodes :
34 35 36
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-38 26-27 27-31 32-33
33-34 35-49 36-37 37-38 39-41 39-40 39-42 42-46 43-49
ring/chain bonds :
34-35 35-36
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26 43-44 43-48 44-45 45-46
46-47 47-48
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-38 26-27 27-31 32-33 33-34 34-35 35-36 35-49 36-37
37-38 39-41 39-40 39-42 42-46 43-44 43-48 43-49 44-45 45-46 46-47
47-48

G1:H,SO3H

G2:O,S,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
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44:CLASS

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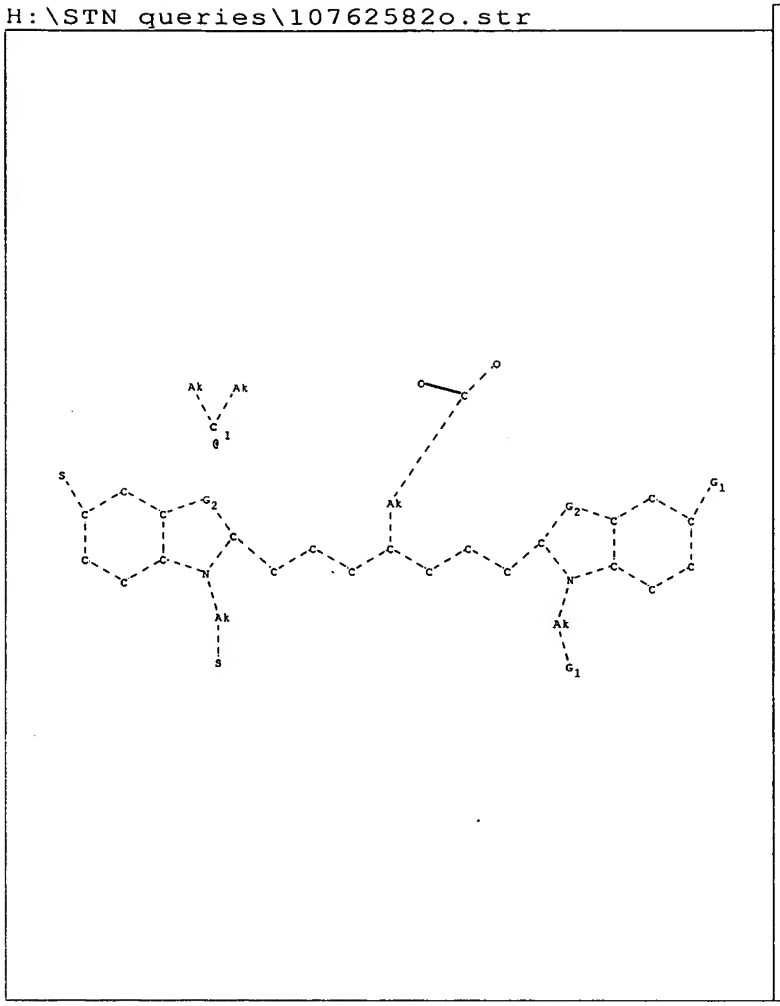

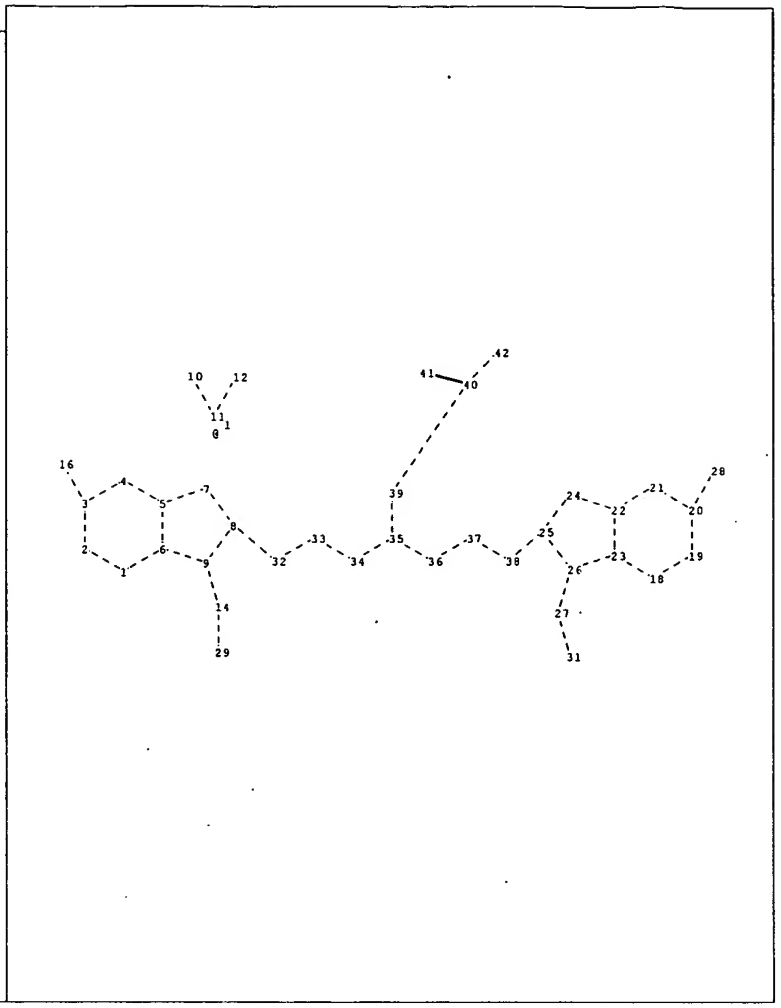

chain nodes :
10 11 12 14 16 27 28 29 31 32 33 37 38 39 40 41 42
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26
ring/chain nodes :
34 35 36
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-38 26-27 27-31 32-33
33-34 35-39 36-37 37-38 39-40 40-42 40-41
ring/chain bonds :
34-35 35-36
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-38 26-27 27-31 32-33 33-34 34-35 35-36 35-39 36-37
37-38 39-40 40-42 40-41

G1:H,SO3H

G2:O,S,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
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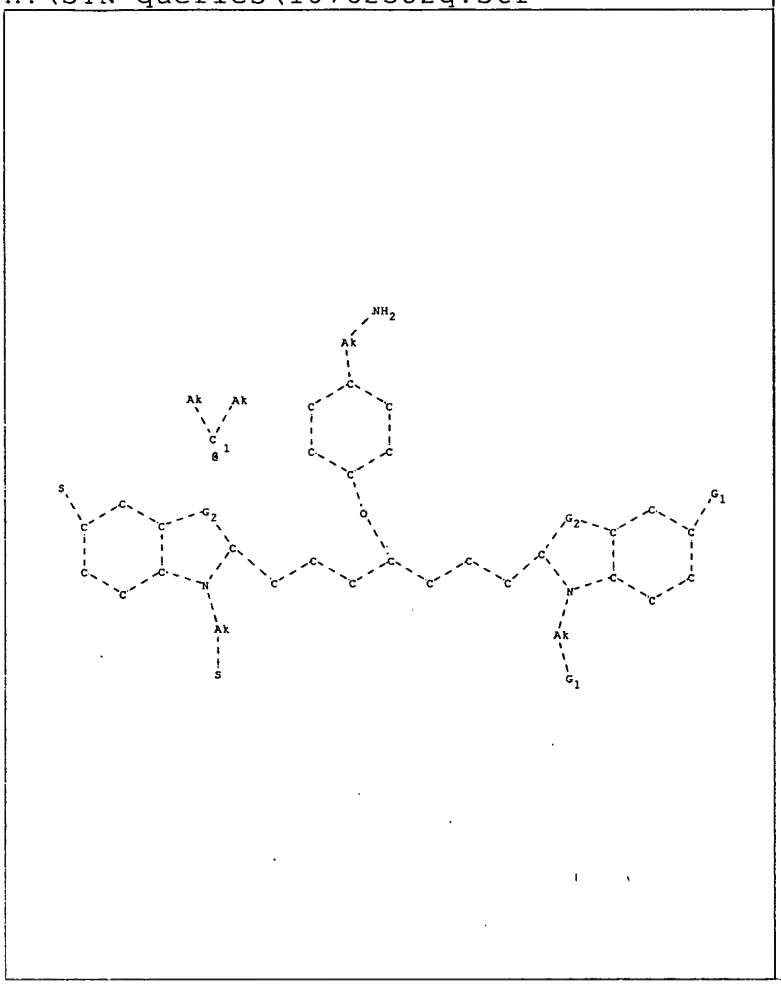

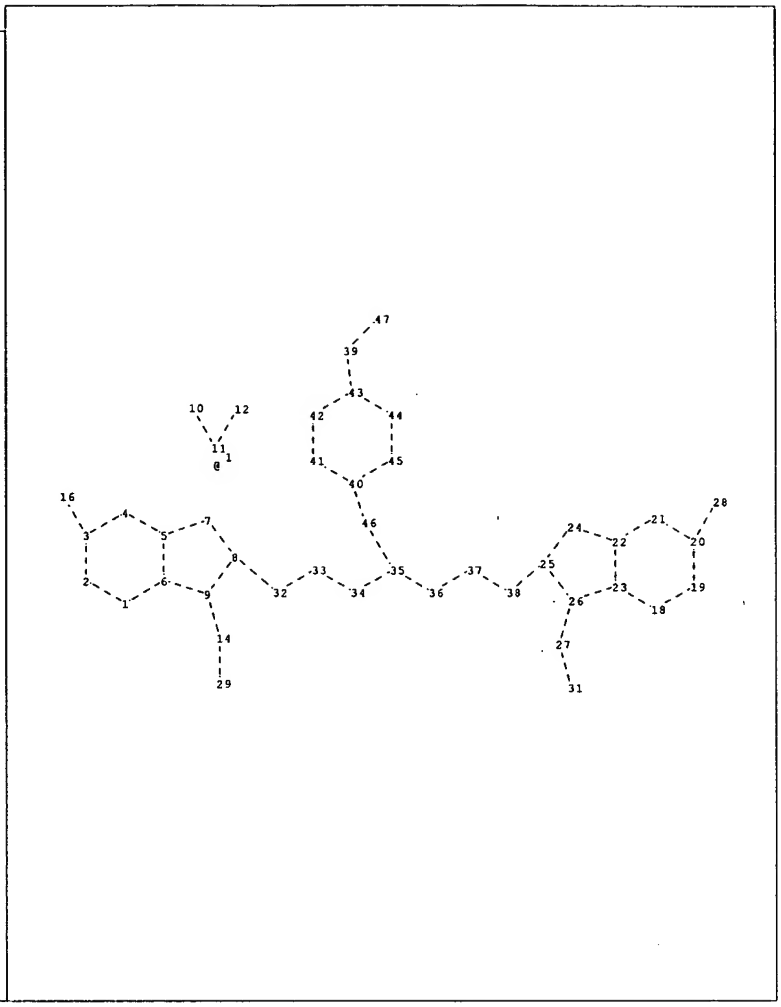

chain nodes :
10 11 12 14 16 27 28 29 31 32 33 37 38 39 46 47
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26 40 41 42
43 44 45
ring/chain nodes :
34 35 36
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-38 26-27 27-31 32-33
33-34 35-46 36-37 37-38 39-43 39-47 40-46
ring/chain bonds :
34-35 35-36
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26 40-41 40-45 41-42 42-43
43-44 44-45
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
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37-38 39-43 39-47 40-41 40-45 40-46 41-42 42-43 43-44 44-45

G1:H,SO3H

G2:O,S,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
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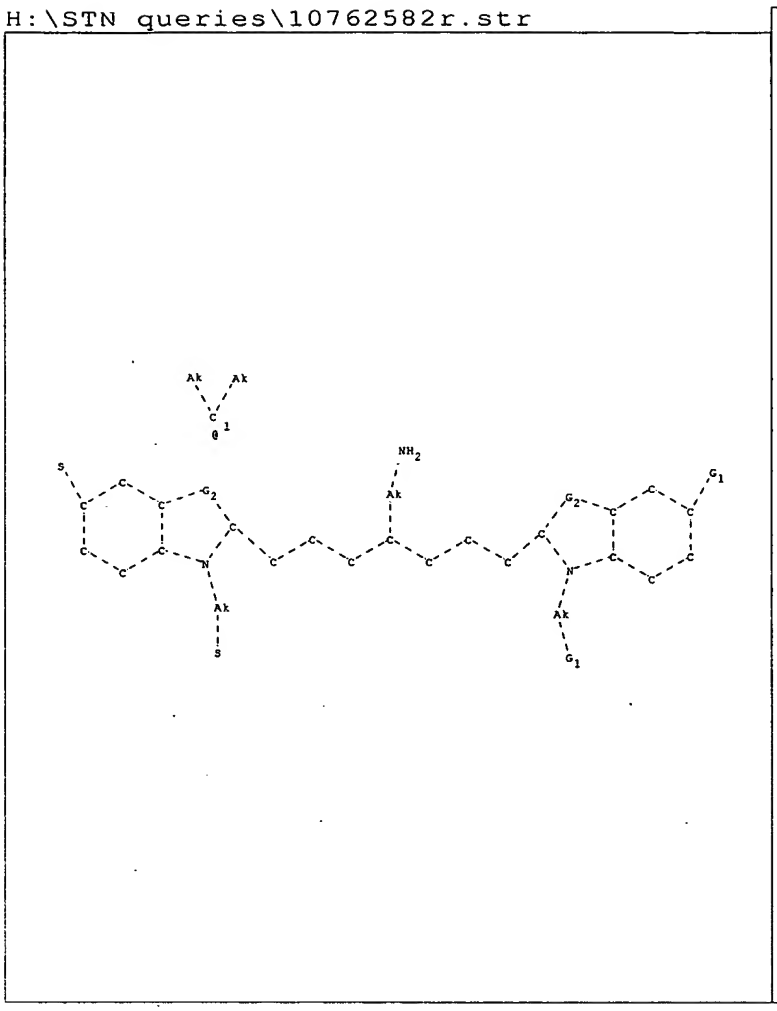

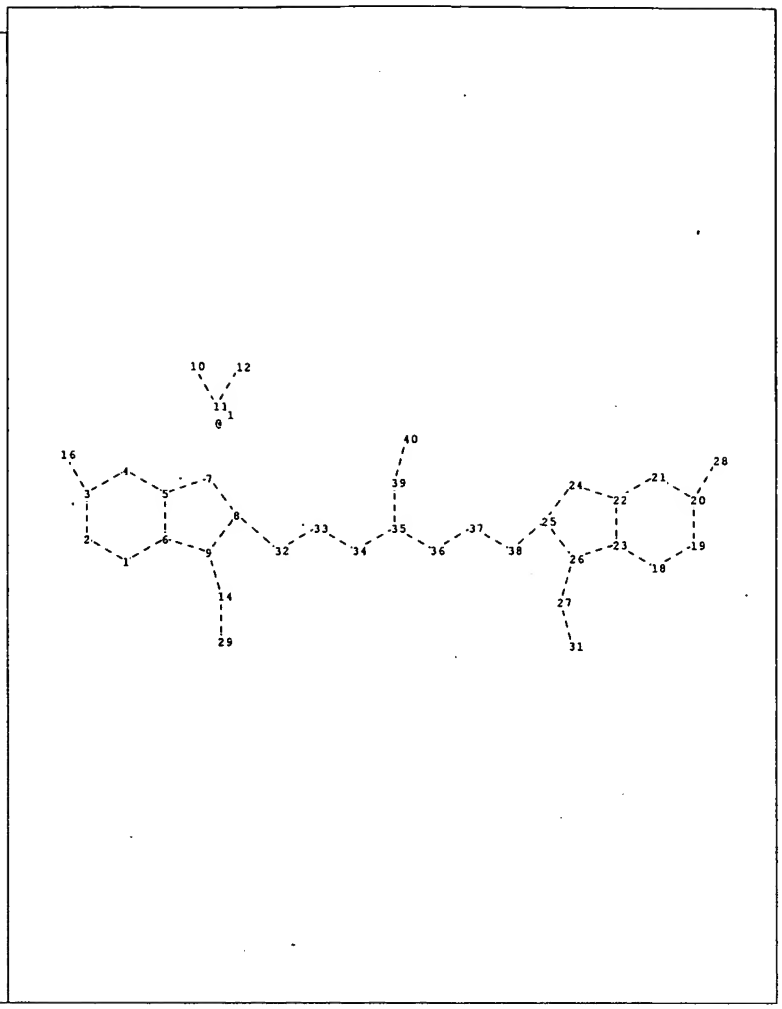

chain nodes :
10 11 12 14 16 27 28 29 31 32 33 37 38 39 40
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26
ring/chain nodes :
34 35 36
chain bonds :
3-16 8-32 9-14 10-11 11-12 14-29 20-28 25-38 26-27 27-31 32-33
33-34 35-39 36-37 37-38 39-40
ring/chain bonds :
34-35 35-36
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20
20-21 21-22 22-23 22-24 23-26 24-25 25-26
exact/norm bonds :
1-2 1-6 2-3 3-4 3-16 4-5 5-6 5-7 6-9 7-8 8-9 8-32 9-14 10-11
11-12 14-29 18-19 18-23 19-20 20-21 20-28 21-22 22-23 22-24 23-26
24-25 25-26 25-38 26-27 27-31 32-33 33-34 34-35 35-36 35-39 36-37
37-38 39-40

G1:H,SO3H

G2:O,S,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 14:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
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37:CLASS 38:CLASS 39:CLASS 40:CLASS

L32 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:633995 HCAPLUS
DOCUMENT NUMBER: 141:158512
TITLE: Hydrophilic, thiol-reactive cyanine dyes and conjugates thereof with biomolecules for fluorescence diagnosis
INVENTOR(S): Licha, Kai; Perlitz, Christin
PATENT ASSIGNEE(S): Schering Ag, Germany
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004065491	A1	20040805	WO 2003-EP12735	20031114 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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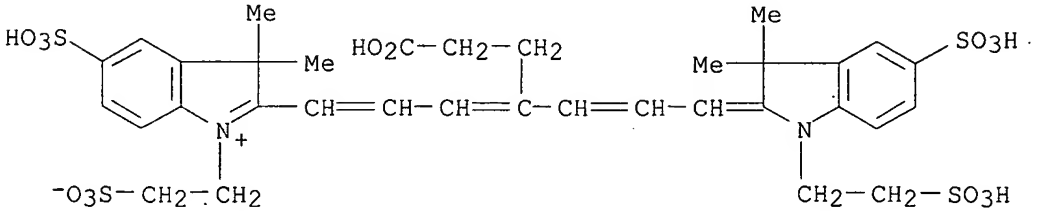
US 2004260072	A1	20041223	US 2004-762582	20040123 <--
PRIORITY APPLN. INFO.:			DE 2003-10302787 A	20030124 <--
			US 2003-443197P P	20030129

OTHER SOURCE(S): MARPAT 141:158512
IT **731862-91-2P 731862-98-9P 731863-01-7P**
731863-04-0P 731863-05-1P 731863-06-2P
731863-08-4P 731863-09-5P 731863-10-8P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of hydrophilic, thiol-reactive cyanine dyes and conjugates thereof with biomols. for fluorescence diagnosis)
RN 731862-91-2 HCAPLUS
CN 3H-Indolium, 2-[4-(2-carboxyethyl)-7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



●3 Na

RN 731862-98-9 HCAPLUS
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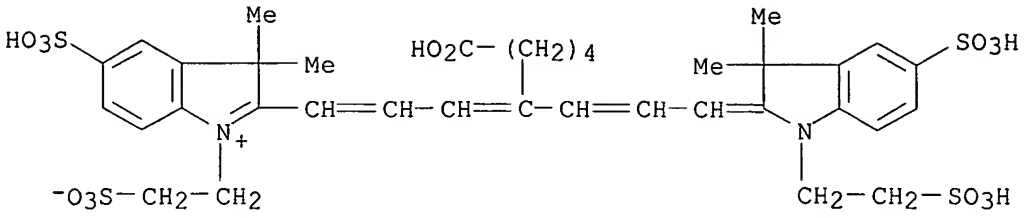
sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



●3 Na

RN 731863-01-7 HCAPLUS
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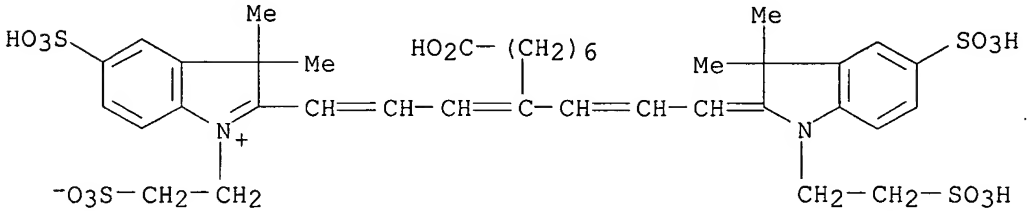

●3 Na

RN 731863-04-0 HCAPLUS
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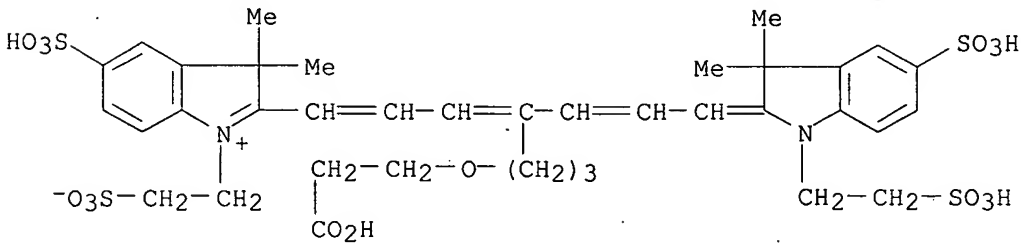

●3 Na

RN 731863-05-1 HCAPLUS
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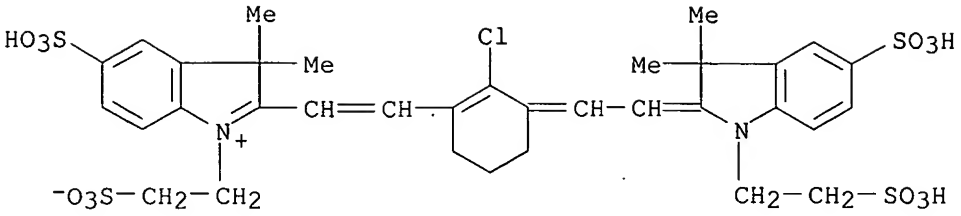

●3 Na

RN 731863-06-2 HCAPLUS
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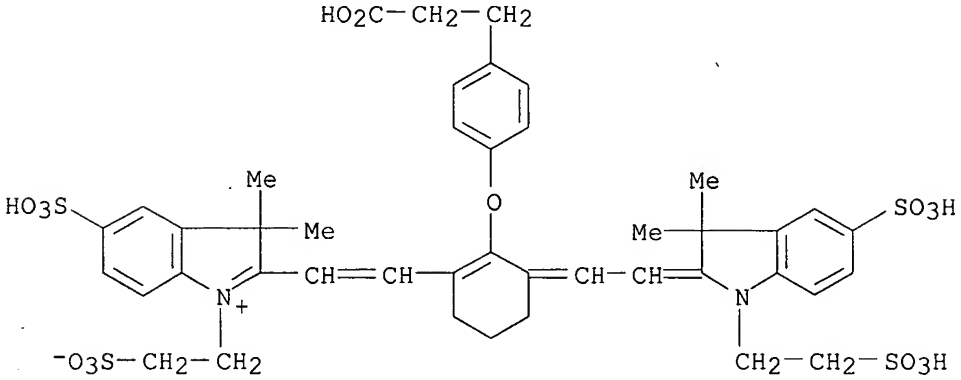
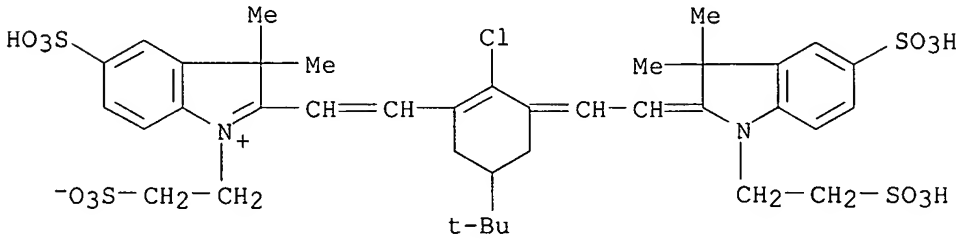


●3 Na

RN 731863-08-4 HCAPLUS
CN 3H-Indolium, 2-[2-[2-chloro-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-5-(1,1-dimethylethyl)-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



●3 Na

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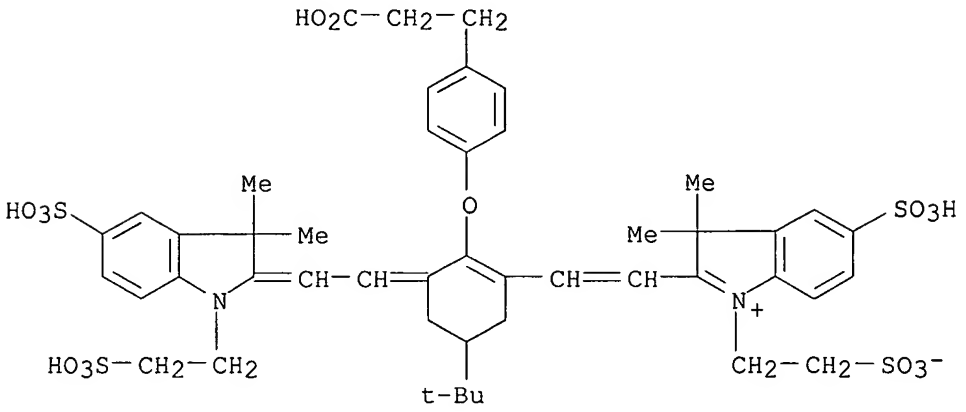

●3 Na

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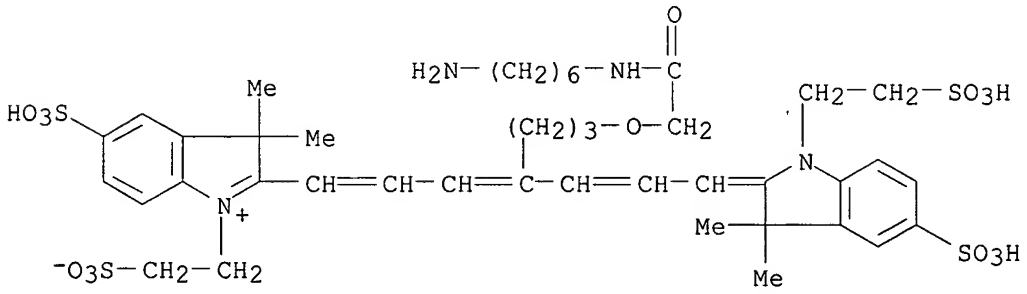
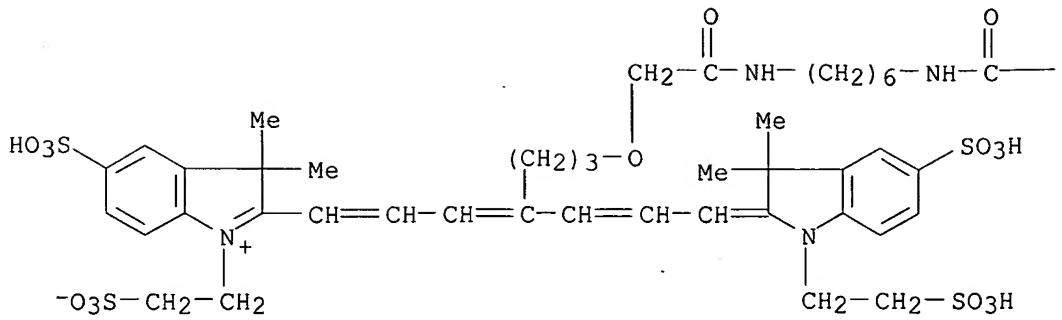


●3 Na

IT **731862-87-6P**
RL: IMF (Industrial manufacture); RCT (Reactant); RGT (Reagent); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of hydrophilic, thiol-reactive cyanine dyes and conjugates thereof with biomols. for fluorescence diagnosis)

RN 731862-87-6 HCAPLUS
CN 3H-Indolium, 2-[4-[3-[2-[[6-[(bromoacetyl)amino]hexyl]amino]-2-oxoethoxy]propyl]-7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



● 3 Na

PAGE 1-B

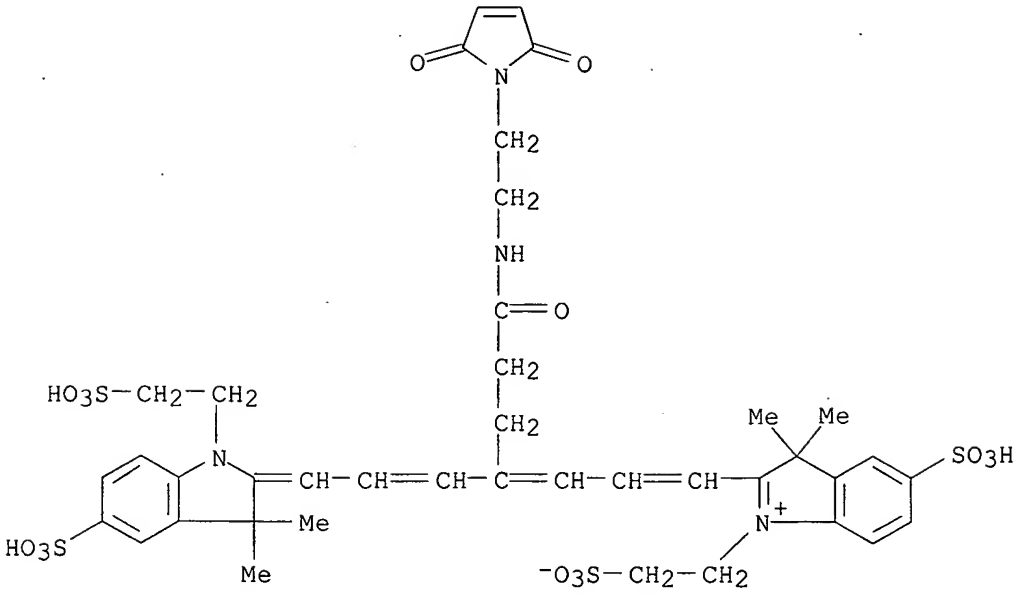
— CH_2Br

IT **731862-71-8P 731862-72-9P 731862-73-0P**
731862-74-1P 731862-75-2P 731862-76-3P
731862-77-4P 731862-78-5P 731862-79-6P
731862-80-9P 731862-81-0P 731862-82-1P
731862-83-2P 731862-84-3P 731862-85-4P
731862-86-5P 731862-88-7P
RL: IMF (Industrial manufacture); RGT (Reagent); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of hydrophilic, thiol-reactive cyanine dyes and conjugates thereof with biomols. for fluorescence diagnosis)

RN 731862-71-8 HCAPLUS

CN 3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-4-[3-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-3-oxopropyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

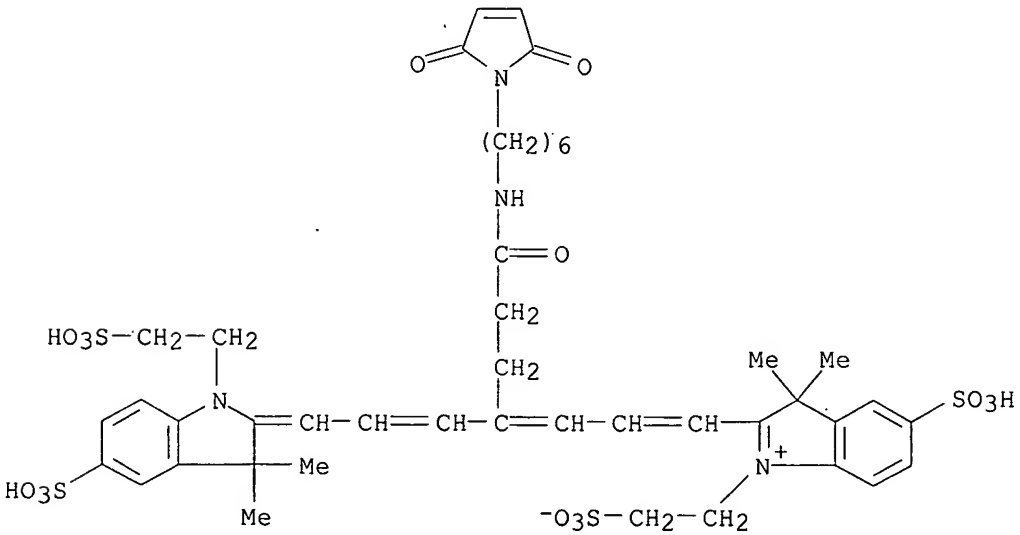


PAGE 2-A

●3 Na

RN 731862-72-9 HCAPLUS
CN 3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-4-[3-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexyl]amino]-3-oxopropyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

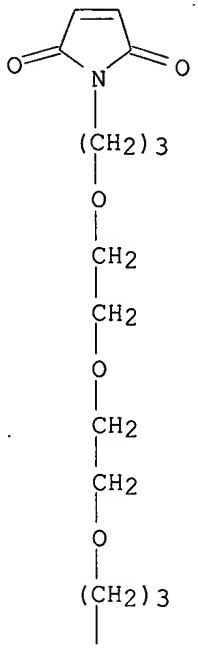


PAGE 2-A

●3 Na

RN 731862-73-0 HCAPLUS
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-21-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-7-oxo-12,15,18-trioxa-8-azaheneicosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



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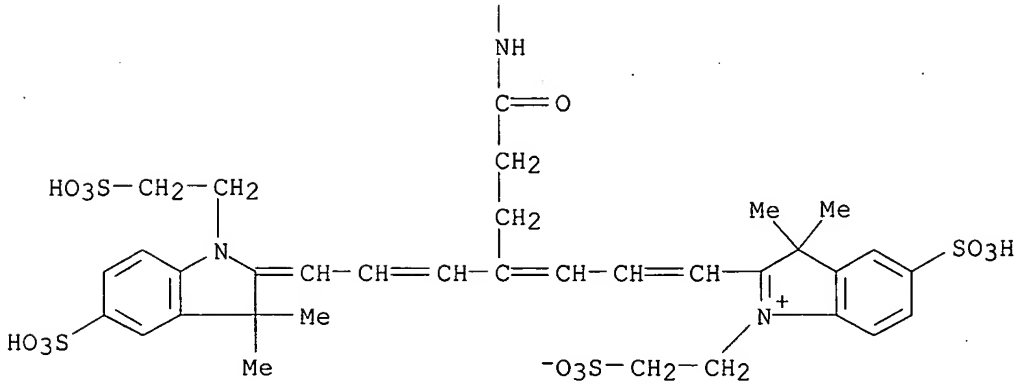
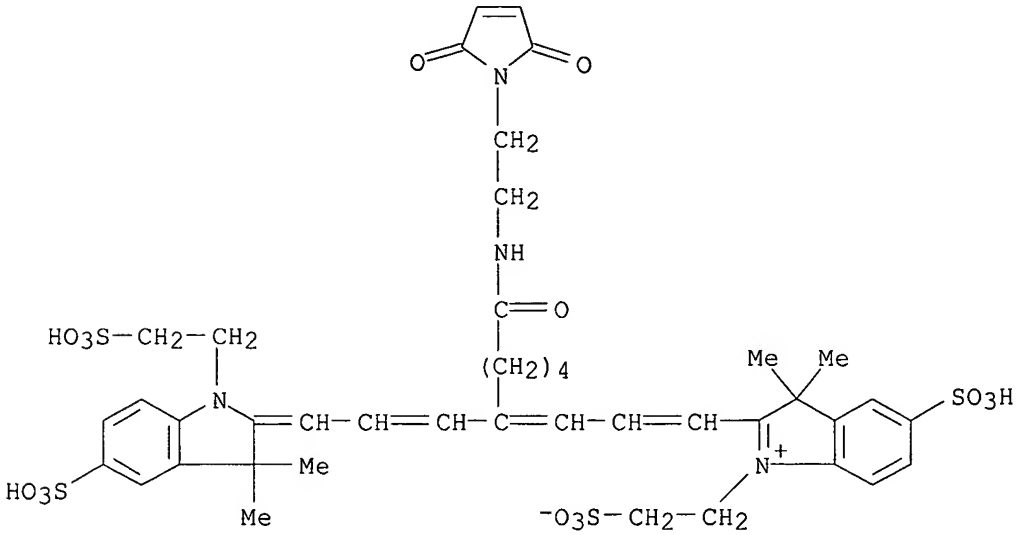


●3 Na

RN 731862-74-1 HCAPLUS

CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-9-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-9-oxo-1,3-nonadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

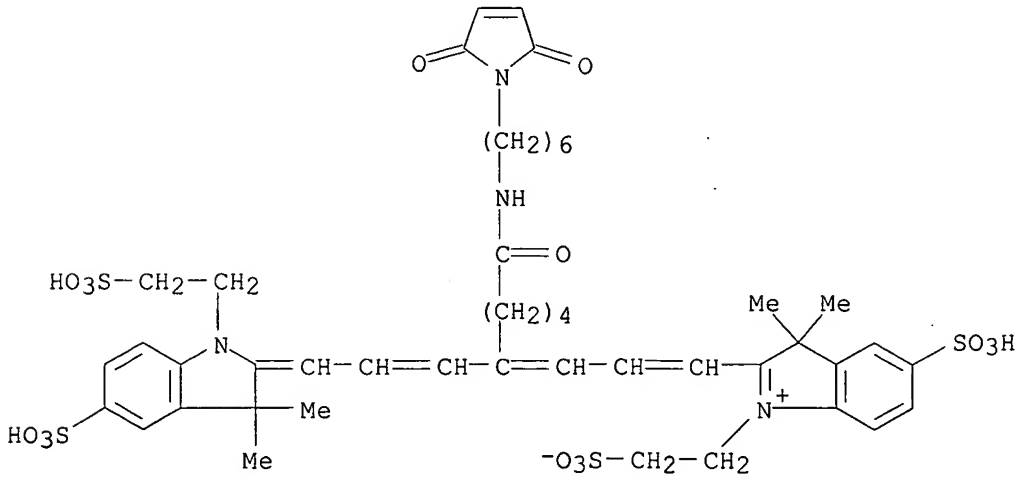
PAGE 1-A



PAGE 2-A

●3 Na

RN 731862-75-2 HCAPLUS
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-9-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexyl]amino]-9-oxo-1,3-nonadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



●3 Na

RN 731862-76-3 HCAPLUS
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-23-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-9-oxo-14,17,20-trioxa-10-azatricosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

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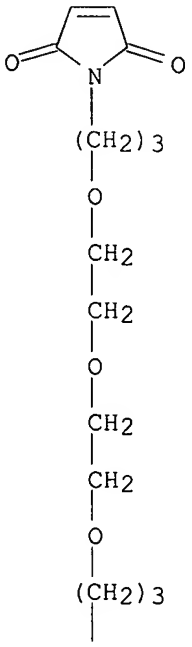

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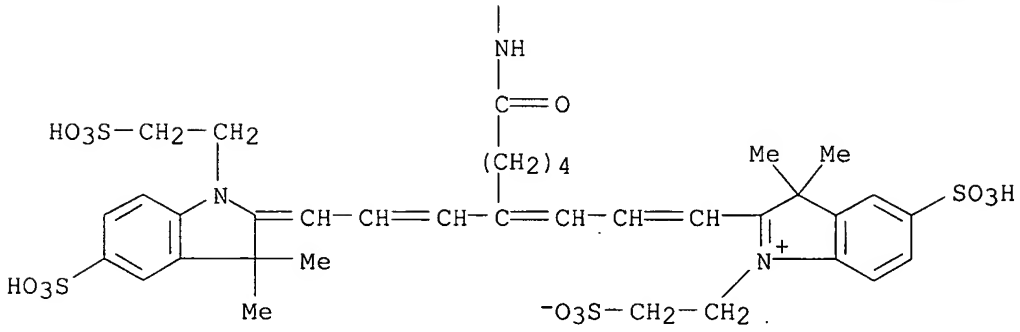
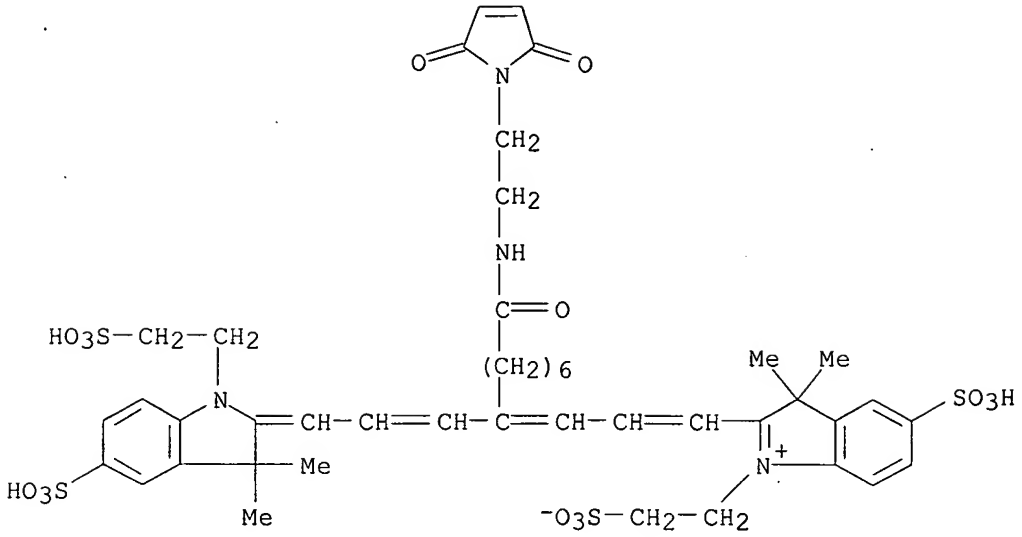


●3 Na

RN 731862-77-4 HCAPLUS
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-11-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-11-oxo-1,3-undecadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

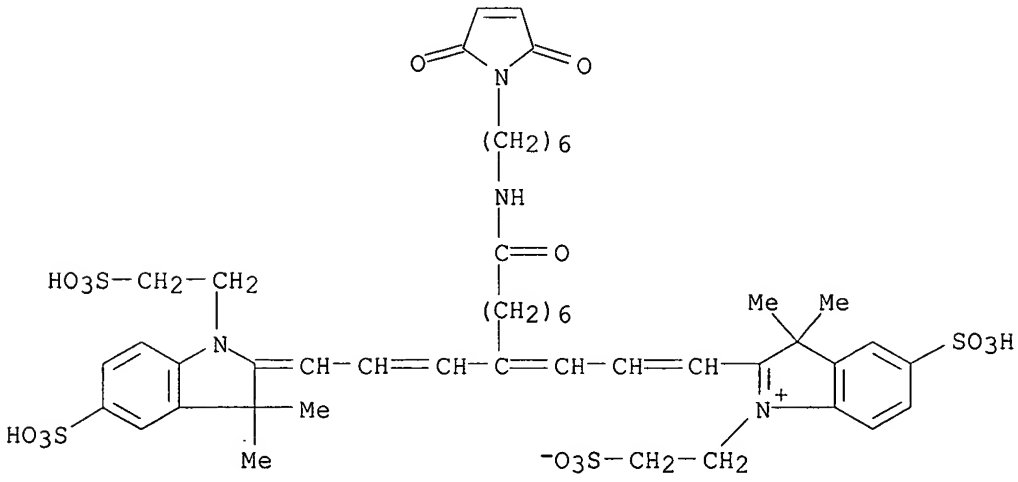
PAGE 1-A



PAGE 2-A

●3 Na

RN 731862-78-5 HCAPLUS
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-11-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexyl]amino]-11-oxo-1,3-undecadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



●3 Na

RN 731862-79-6 HCAPLUS
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-25-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-11-oxo-16,19,22-trioxa-12-azapentacosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

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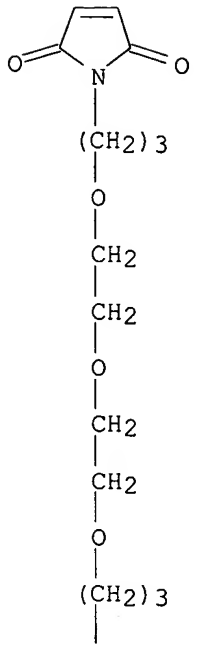

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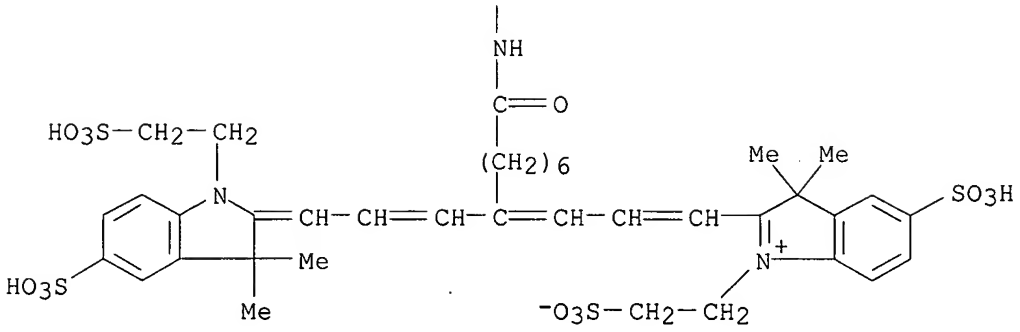
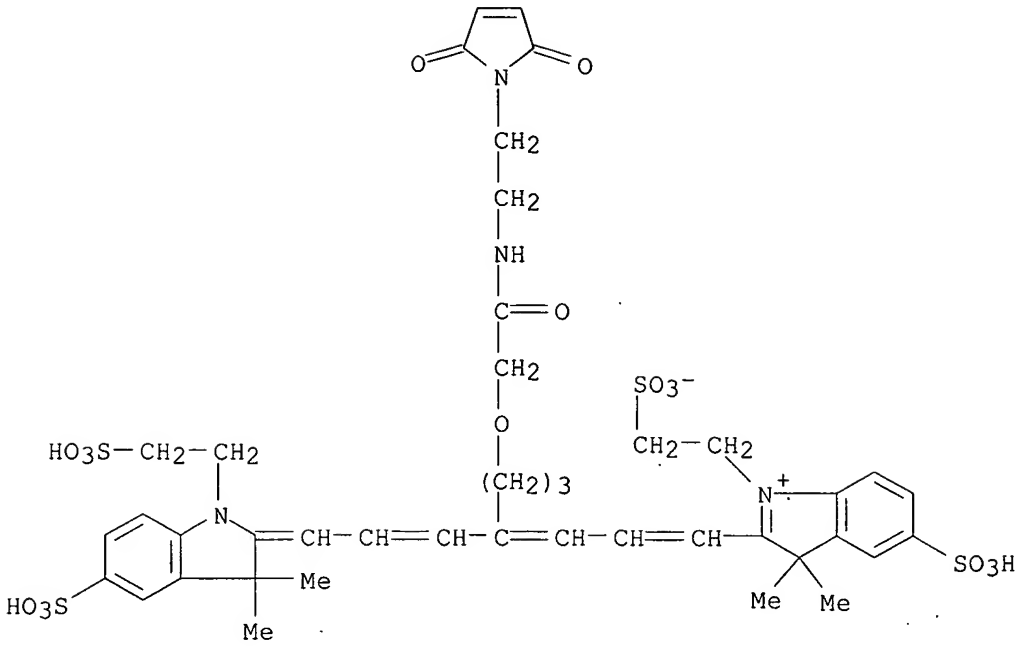


●3 Na

RN 731862-80-9 HCAPLUS
CN 3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-4-[3-[2-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-2-oxoethoxy]propyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

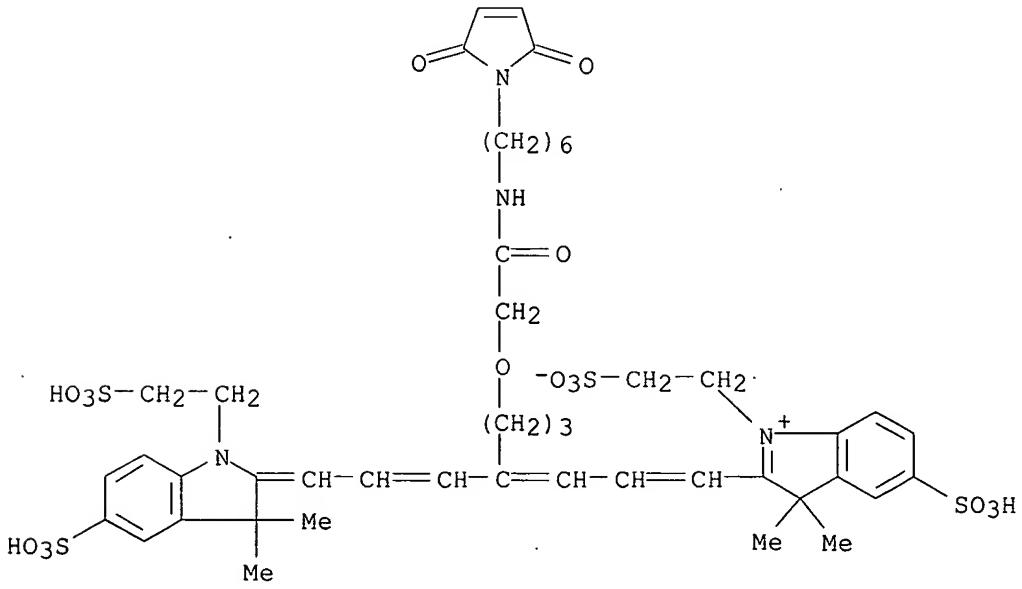


PAGE 2-A

●3 Na

RN 731862-81-0 HCAPLUS
CN 3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-4-[3-[2-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexyl]amino]-2-oxoethoxy]propyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



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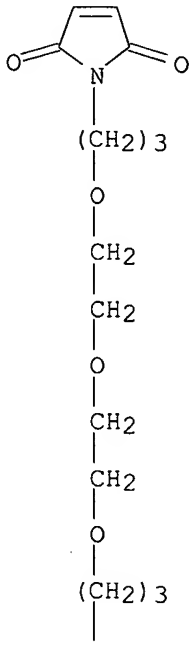
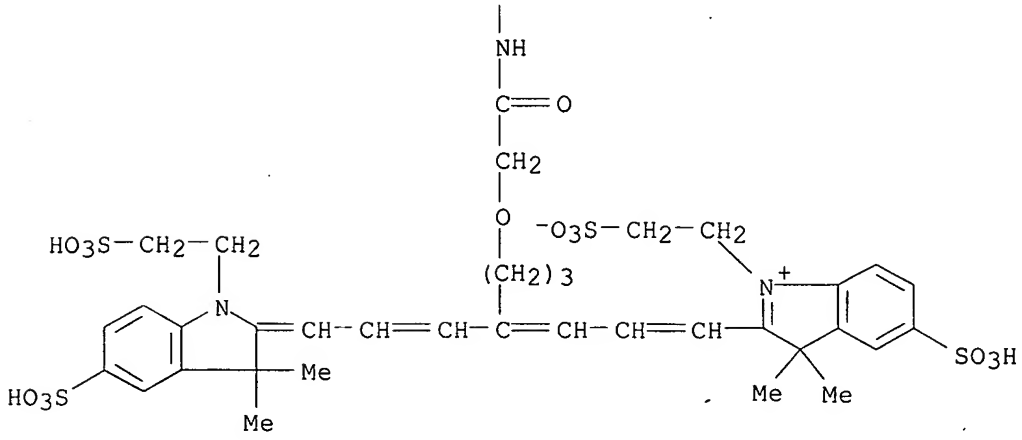
●3 Na

RN 731862-82-1 HCAPLUS
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-24-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-10-oxo-8,15,18,21-tetraoxa-11-azatetracosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



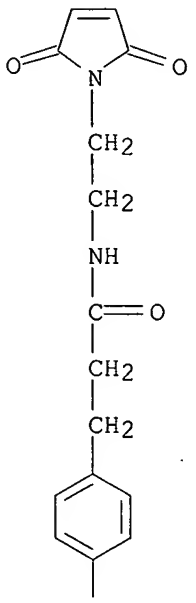
PAGE 2-A



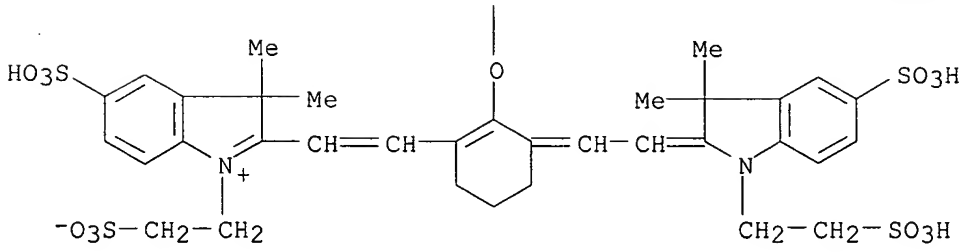
●3 Na

RN 731862-83-2 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



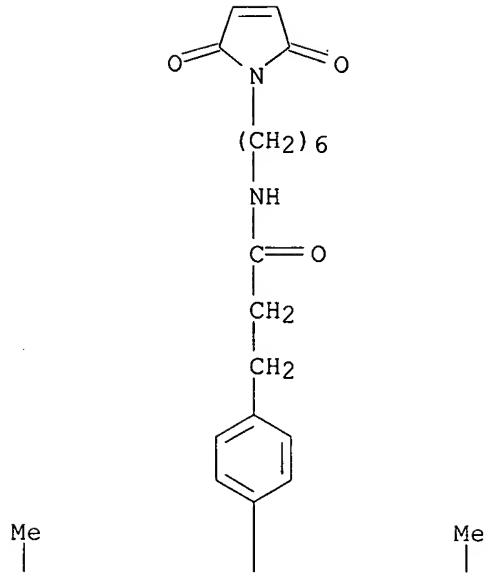
PAGE 2-A



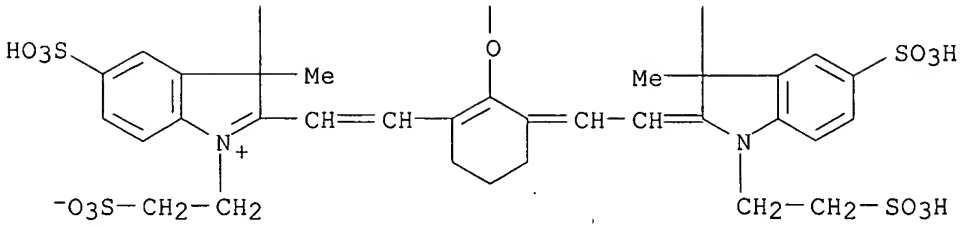
●3 Na

RN 731862-84-3 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexyl]amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



●3 Na

RN 731862-85-4 HCAPLUS

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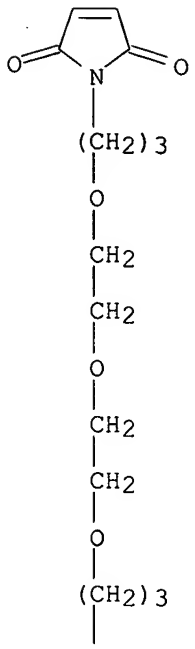
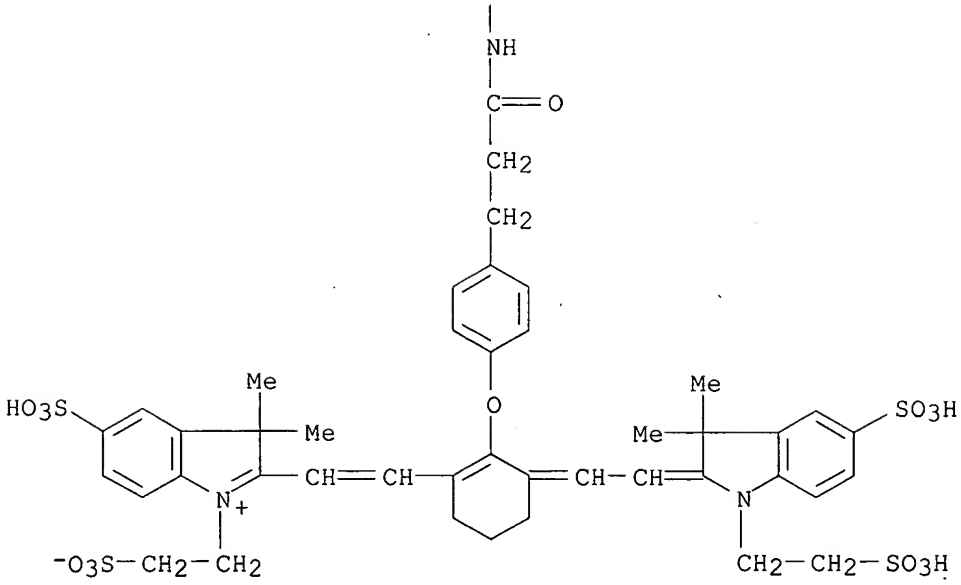
PAGE 1-A



PAGE 2-A



PAGE 3-A

●3 Na

RN 731862-86-5 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-3-oxopropyl]phenoxy]-5-(1,1-dimethylethyl)-1-

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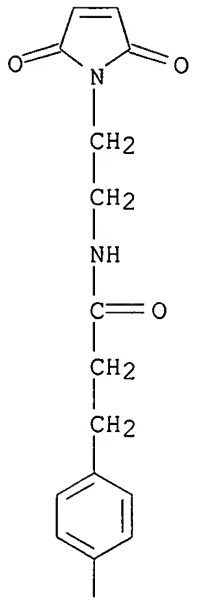
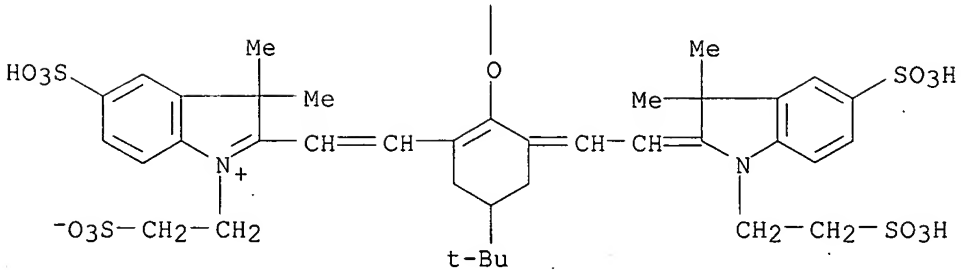
PAGE 1-A



PAGE 2-A



●3 Na

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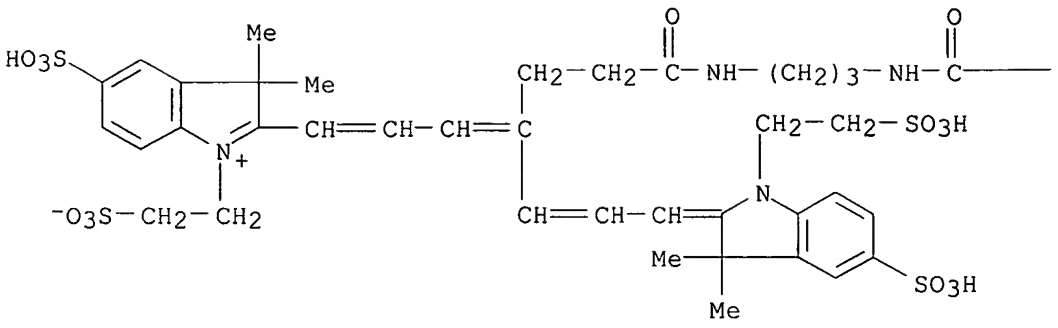
PAGE 1-A



●3 Na

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— CH_2Br

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:485574 HCAPLUS
DOCUMENT NUMBER: 141:20106
TITLE: In vivo imaging of apoptosis using fluorochromes conjugated to annexin A5 or synaptotagmin
INVENTOR(S): Bogdanov, Alexei; Schellenberger, Eyk; Petrovsky, Alexander; Josephson, Lee
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 24 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004022731	A1	20040205	US 2003-424232	20030425 <--
CA 2479938	AA	20031224	CA 2003-2479938	20030428 <--
WO 2003105814	A1	20031224	WO 2003-US13494	20030428 <--
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1499292	A1	20050126	EP 2003-728626	20030428 <--
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JP 2005523945	T2	20050811	JP 2004-512720	20030428 <--

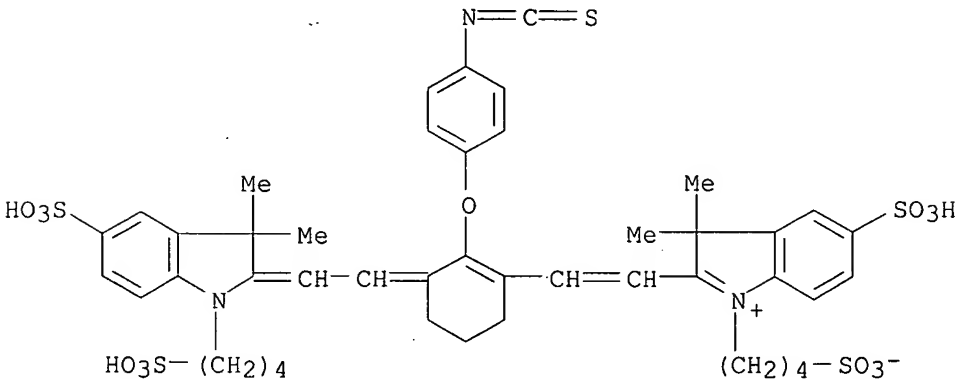
PRIORITY APPLN. INFO.:

US 2002-376052P	P	20020426 <--
US 2003-424232	A	20030425
WO 2003-US13494	W	20030428

IT **166547-11-1D**, IRDye-38, conjugates **398142-13-7D**, IRDye-78, conjugates
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(in vivo imaging of apoptosis using fluorochromes conjugated to annexin A5 or synaptotagmin)

RN 166547-11-1 HCAPLUS

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-(4-isothiocyanatophenoxy)-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



●3 Na

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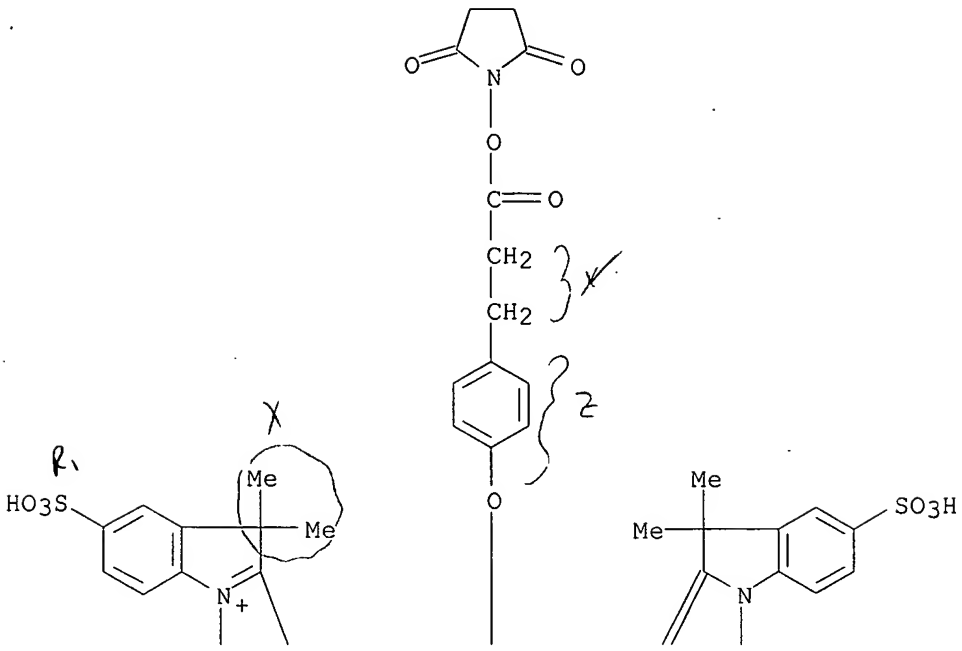
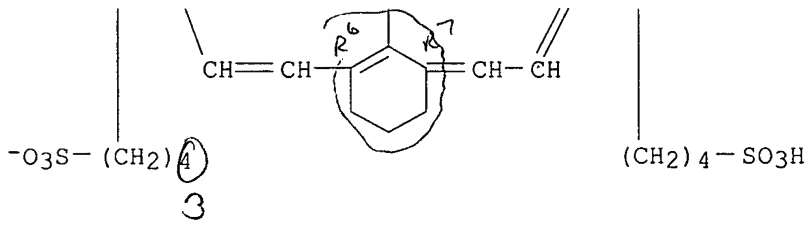
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



●3 Na

L32 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:60345 HCAPLUS
DOCUMENT NUMBER: 140:124836
TITLE: Conjugated infrared fluorescent substances for detection of cell death
INVENTOR(S): Frangioni, John V.
PATENT ASSIGNEE(S): Beth Israel Deaconess Medical Center, USA
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004006963	A1	20040122	WO 2003-US21478	20030710 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

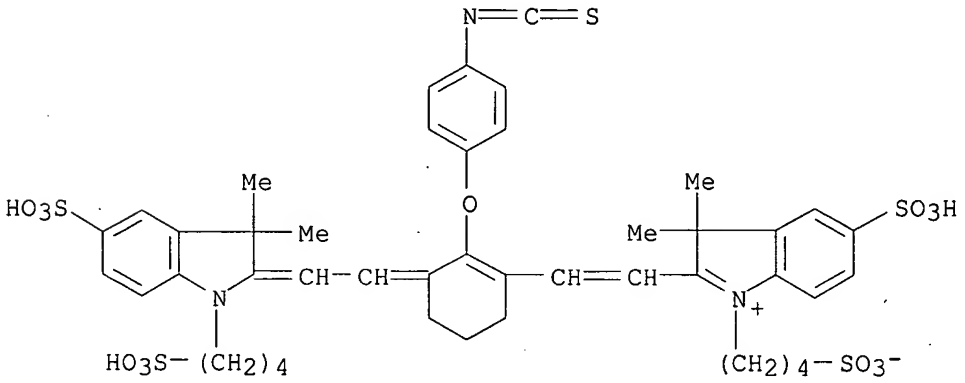
PRIORITY APPLN. INFO.: US 2002-395582P P 20020712 <--

OTHER SOURCE(S): MARPAT 140:124836

IT **166547-11-1D**, IRDye 38, conjugates with cell death-targeting agent
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); DGN (Diagnostic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(IRDye 38; targeting conjugated IR fluorescent substances for detection of cell death)

RN 166547-11-1 HCAPLUS

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-(4-isothiocyanatophenoxy)-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



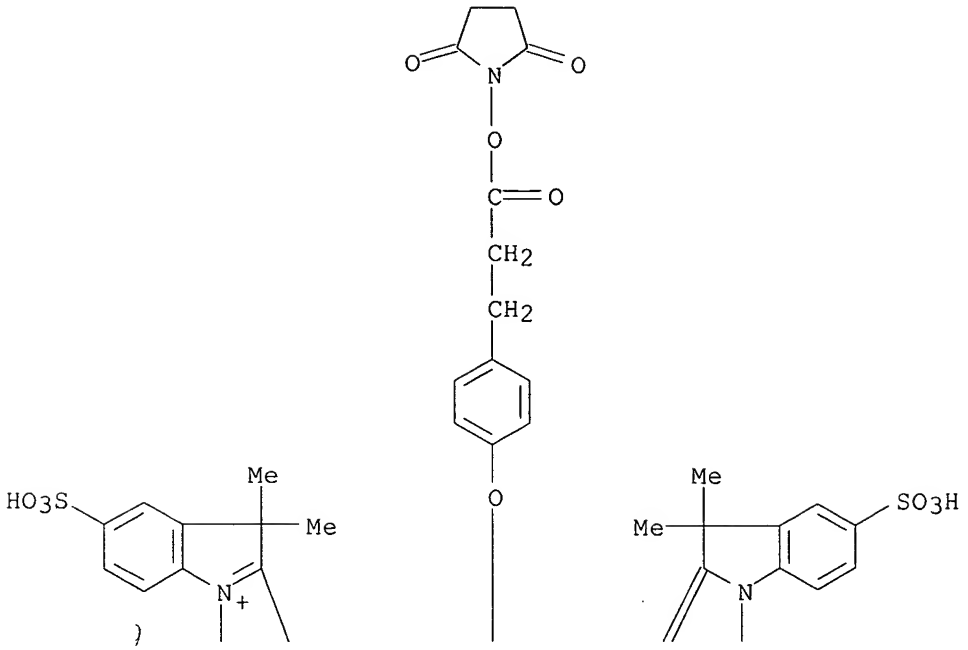
●3 Na

IT **398142-13-7D**, IRDye 78, conjugates with annexin V
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); DGN (Diagnostic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(targeting conjugated IR fluorescent substances for detection of cell death)

RN 398142-13-7 HCAPLUS

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



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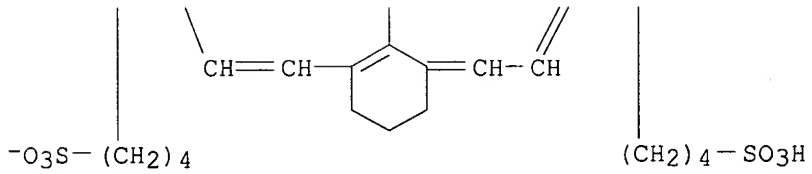

●3 Na

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:470344 HCAPLUS
DOCUMENT NUMBER: 139:48112
TITLE: High throughput analysis and detection of multiple target nucleotide sequences such as single nucleotide polymorphisms
INVENTOR(S): Van Eijk, Michael J. T.
PATENT ASSIGNEE(S): Keygene N.V., Neth.
SOURCE: Eur. Pat. Appl., 63 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1319718	A1	20030618	EP 2001-204912	20011214

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

CA 2470356 AA 20030626 CA 2002-2470356 20021216 <--

WO 2003052140 A2 20030626 WO 2002-NL832 20021216 <--

WO 2003052140 A3 20031113

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

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WO 2003052141 A2 20030626 WO 2002-NL833 20021216 <--

WO 2003052141 C2 20031218

WO 2003052141 A3 20040226

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

WO 2003052142 A2 20030626 WO 2002-NL834 20021216 <--

WO 2003052142 A3 20031030

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1453978 A2 20040908 EP 2002-795451 20021216 <--

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

JP 2005512549 T2 20050512 JP 2003-553009 20021216 <--

PRIORITY APPLN. INFO.: EP 2001-204912 A 20011214 <--

WO 2002-NL834 W 20021216 <--

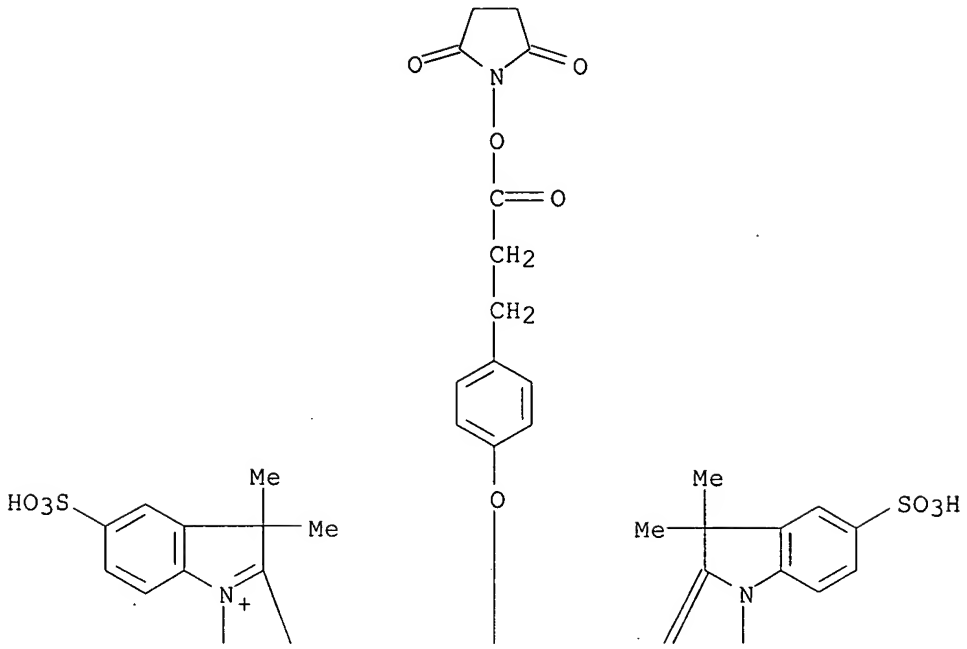
IT **398142-13-7D**, oligonucleotide conjugates

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (IRDye; high throughput anal. and detection of multiple target nucleotide sequences such as single nucleotide polymorphisms)

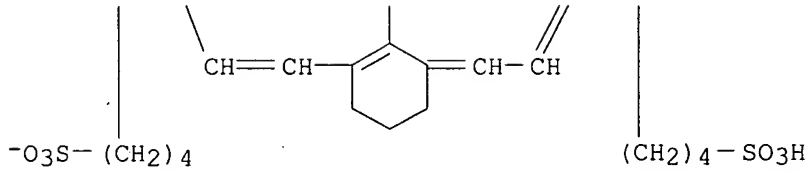
RN 398142-13-7 HCAPLUS

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



●3 Na

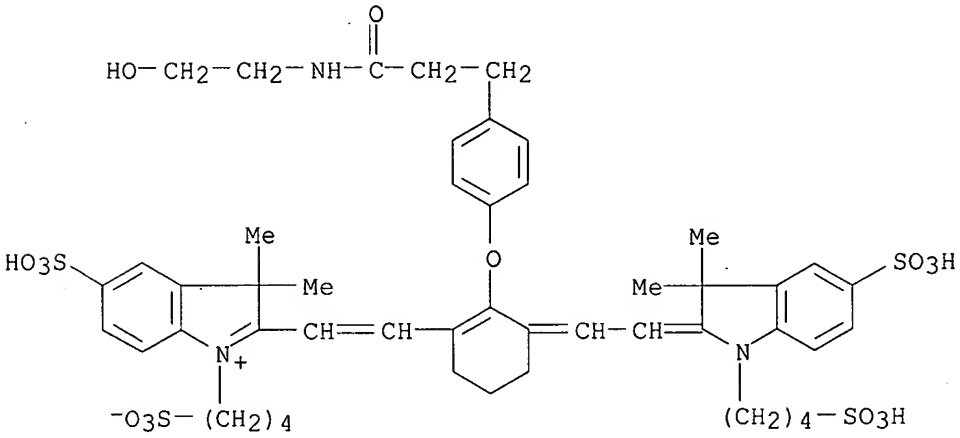
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:65972 HCAPLUS
DOCUMENT NUMBER: 139:288409
TITLE: IRDye78 conjugates for near-infrared fluorescence imaging
AUTHOR(S): Zaheer, Atif; Wheat, Thomas E.; Frangioni, John V.
CORPORATE SOURCE: Beth Israel Deaconess Medical Center, Boston, MA, USA
SOURCE: Molecular Imaging (2002), 1(4), 354-364
CODEN: MIOMBP; ISSN: 1535-3508
PUBLISHER: MIT Press
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **607709-66-0P 607709-68-2P 607709-70-6P**
607709-72-8P 607709-74-0P 607709-76-2P
607709-78-4P
RL: PNU (Preparation, unclassified); PREP (Preparation)
(purification of IRDye78 conjugates by ion-pairing HPLC in relation to applications for near-IR fluorescence imaging)

RN 607709-66-0 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2-hydroxyethyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, compd. with N,N-diethylethanamine (1:3) (9CI) (CA INDEX NAME)

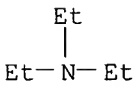
CM 1

CRN 607709-65-9
CMF C49 H61 N3 O15 S4



CM 2

CRN 121-44-8
CMF C6 H15 N



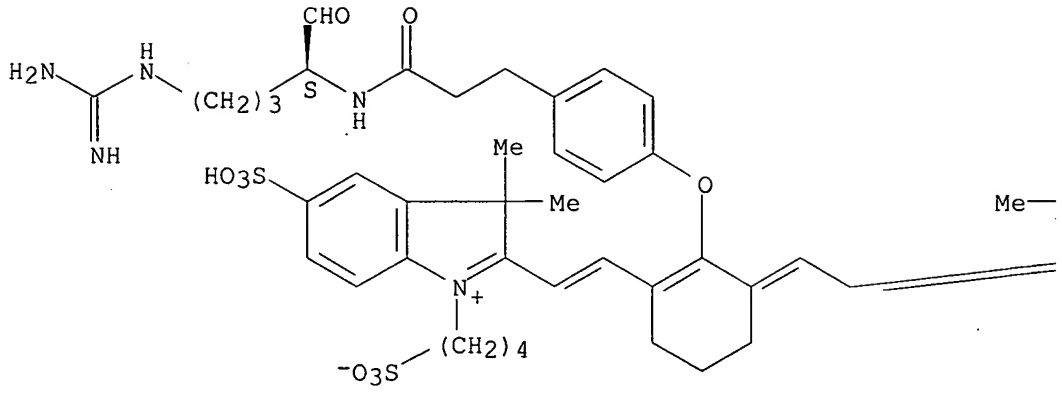
RN 607709-68-2 HCAPLUS
CN 3H-Indolium, 2-[2-[2-[4-[3-[[(1S)-4-[(aminoiminomethyl)amino]-1-formylbutyl]amino]-3-oxopropyl]phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, compd. with N,N-diethylethanamine (1:3) (9CI) (CA INDEX NAME)

CM 1

CRN 607709-67-1
CMF C53 H68 N6 O15 S4

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



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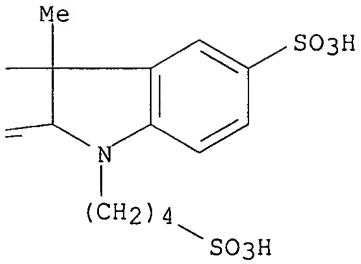
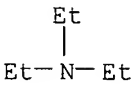


CM 2

CRN 121-44-8
CMF C6 H15 N



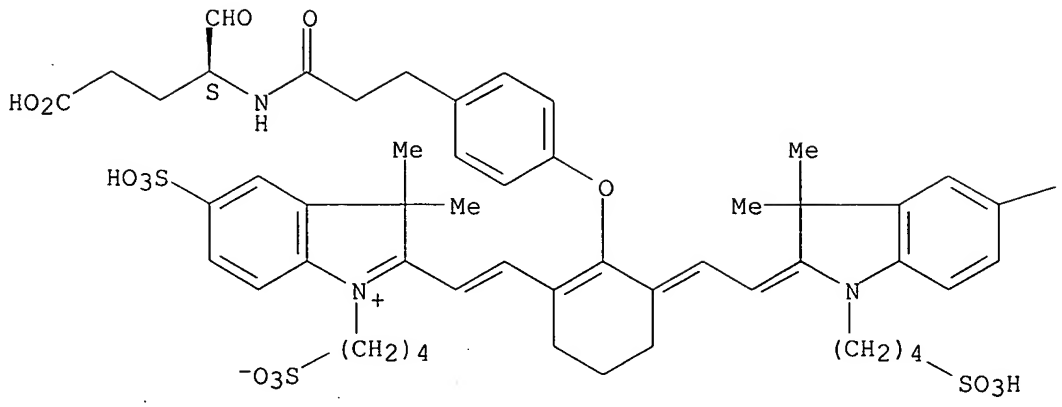
RN 607709-70-6 HCAPLUS
CN 3H-Indolium, 2-[2-[2-[4-[3-[[(1S)-3-carboxy-1-formylpropyl]amino]-3-oxopropyl]phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, compd. with N,N-diethylethanamine (1:3) (9CI) (CA INDEX NAME)

CM 1

CRN 607709-69-3
CMF C52 H63 N3 O17 S4

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A

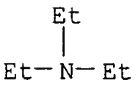


PAGE 1-B

—SO_3H

CM 2

CRN 121-44-8
CMF C6 H15 N



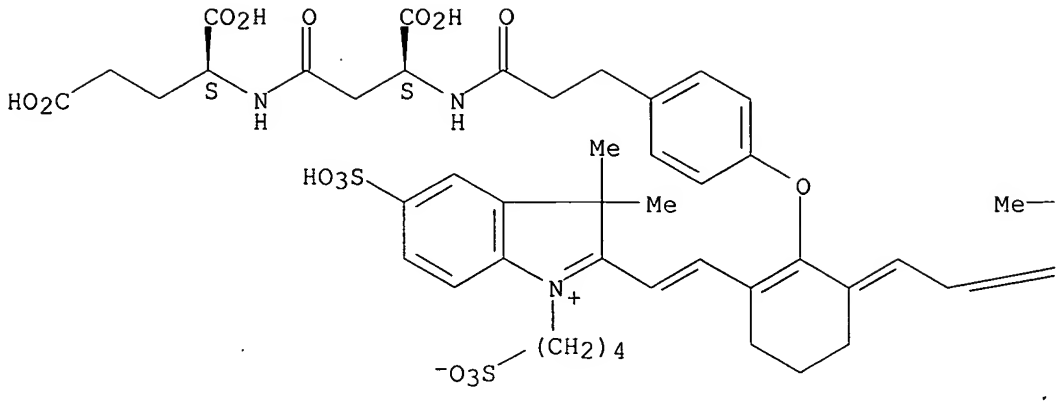
RN 607709-72-8 HCAPLUS
CN L-Glutamic acid, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-oxopropyl]-L-β-aspartyl-, inner salt, compd. with N,N-diethylethanamine (1:3) (9CI) (CA INDEX NAME)

CM 1

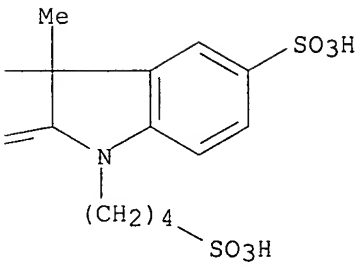
CRN 607709-71-7
CMF C56 H68 N4 O21 S4

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A

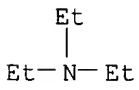


PAGE 1-B



CM 2

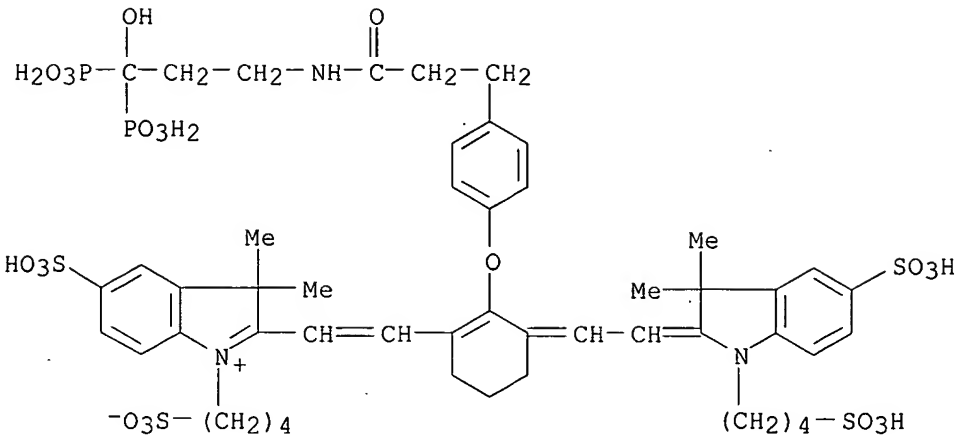
CRN 121-44-8
CMF C6 H15 N



RN 607709-74-0 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(3-hydroxy-3,3-diphosphonopropyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, compd. with N,N-diethylethanamine (1:7) (9CI) (CA INDEX NAME)

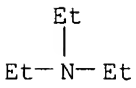
CM 1

CRN 607709-73-9
CMF C50 H65 N3 O21 P2 S4



CM 2

CRN 121-44-8
CMF C6 H15 N



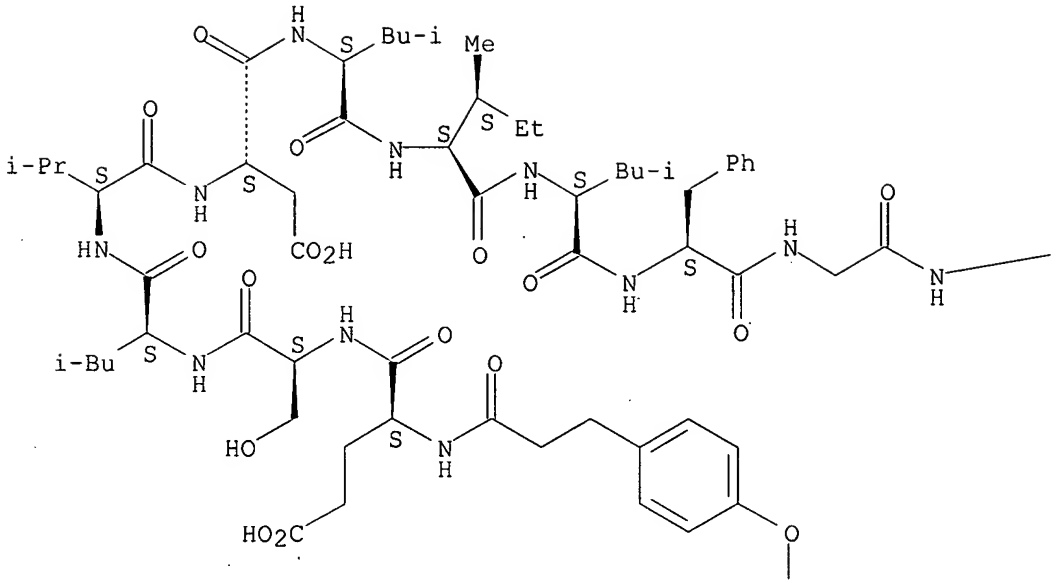
RN 607709-76-2 HCAPLUS
CN L-Serine, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-oxopropyl]-L-α-glutamyl-L-seryl-L-leucyl-L-valyl-L-α-aspartyl-L-leucyl-L-isoleucyl-L-leucyl-L-phenylalanylglycyl-, inner salt, compd. with N,N-diethylethanamine (1:7) (9CI) (CA INDEX NAME)

CM 1

CRN 607709-75-1
CMF C102 H143 N13 O32 S4

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



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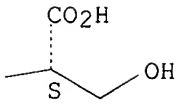

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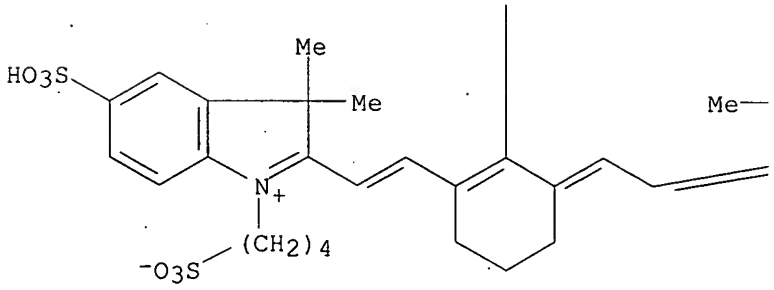
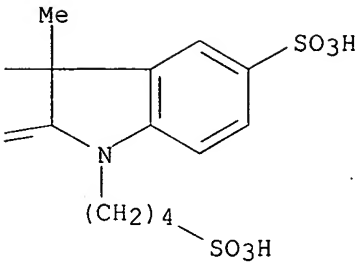
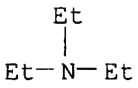




CM 2

CRN 121-44-8
CMF C6 H15 N

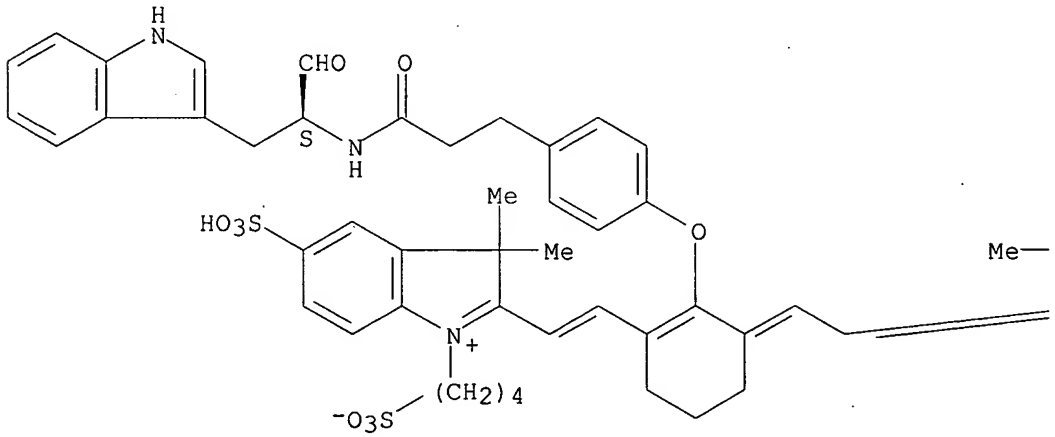


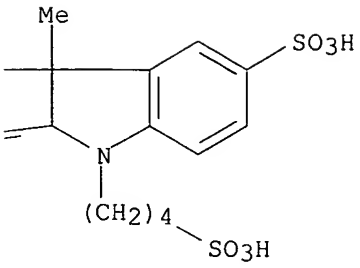
RN 607709-78-4 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[(1S)-1-formyl-2-(1H-indol-3-yl)ethyl]amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, compd. with N,N-diethylethanamine (1:3) (9CI) (CA INDEX NAME)

CM 1

CRN 607709-77-3
CMF C58 H66 N4 O15 S4

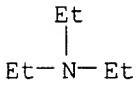
Absolute stereochemistry.
Double bond geometry unknown.





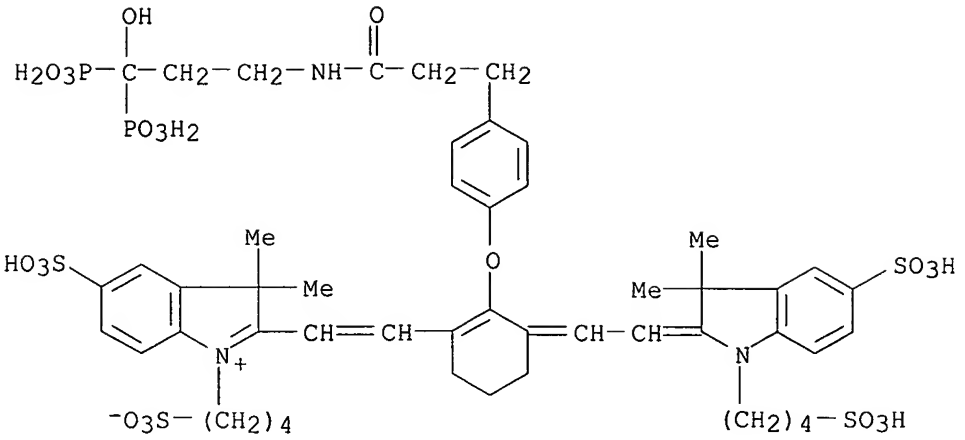
CM 2

CRN 121-44-8
CMF C6 H15 N



IT **397858-89-8P 477808-86-9P 607709-59-1P 607709-60-4P 607709-61-5P 607709-63-7P 607709-64-8P**
RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(purification of IRDye78 conjugates by ion-pairing HPLC in relation to applications for near-IR fluorescence imaging)

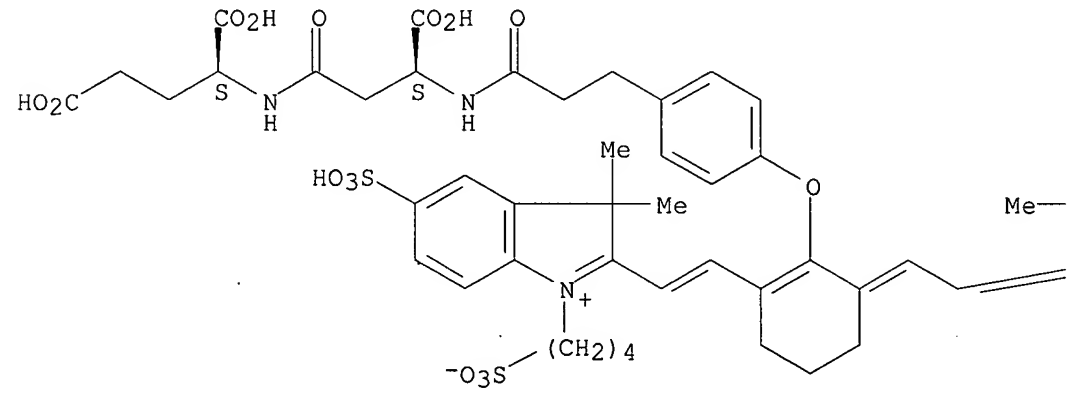
RN 397858-89-8 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(3-hydroxy-3,3-diphosphonopropyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, heptasodium salt (9CI) (CA INDEX NAME)



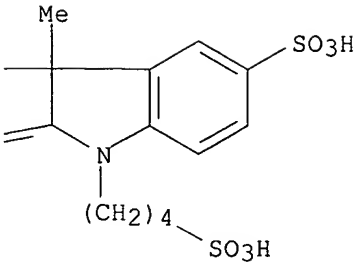
●7 Na

RN 477808-86-9 HCAPLUS
CN L-Glutamic acid, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-oxopropyl]-L-β-aspartyl-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

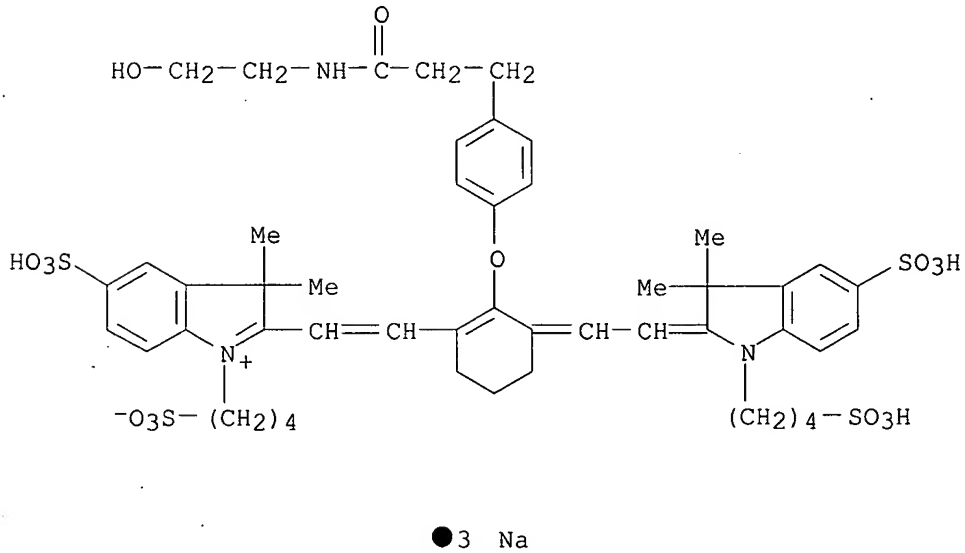
Absolute stereochemistry.
Double bond geometry unknown.



●3 Na



RN 607709-59-1 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2-hydroxyethyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

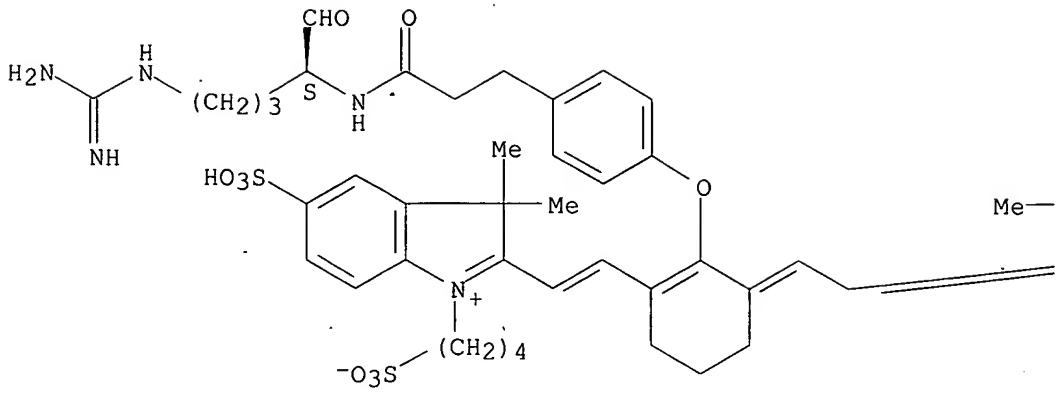


●3 Na

RN 607709-60-4 HCAPLUS
CN 3H-Indolium, 2-[2-[2-[4-[3-[[(1S)-4-[(aminoiminomethyl)amino]-1-formylbutyl]amino]-3-oxopropyl]phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

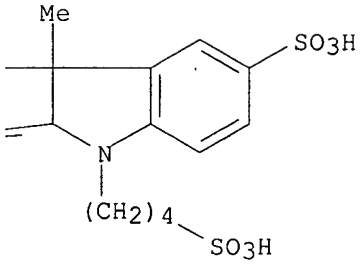
Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



●3 Na

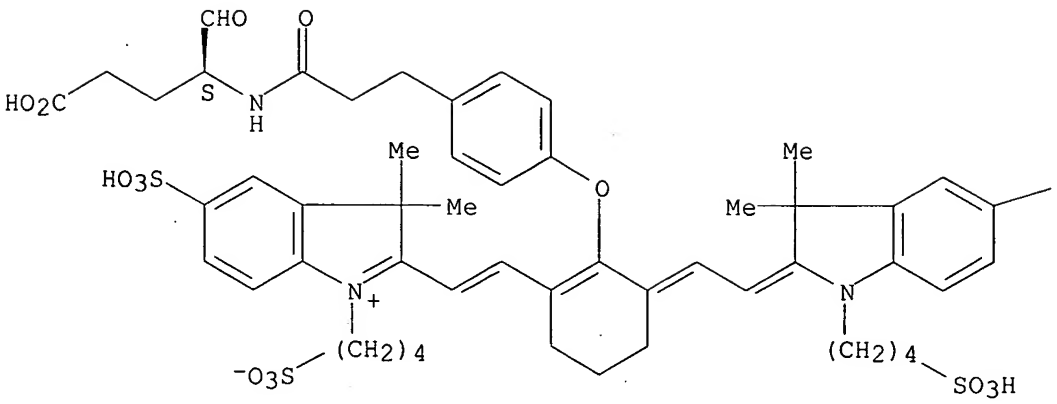
PAGE 1-B



RN 607709-61-5 HCAPLUS
CN 3H-Indolium, 2-[2-[2-[4-[3-[[(1S)-3-carboxy-1-formylpropyl]amino]-3-oxopropyl]phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



●3 Na

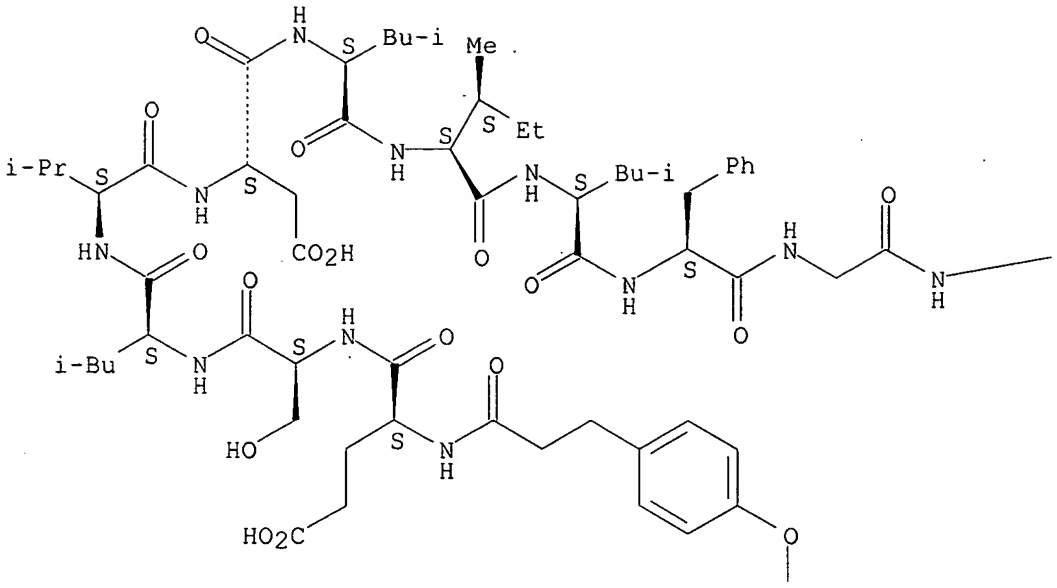
PAGE 1-B

—SO_3H

RN 607709-63-7 HCAPLUS
CN L-Serine, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-oxopropyl]-L-α-glutamyl-L-seryl-L-leucyl-L-valyl-L-α-aspartyl-L-leucyl-L-isoleucyl-L-leucyl-L-phenylalanylglycyl-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



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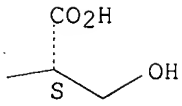

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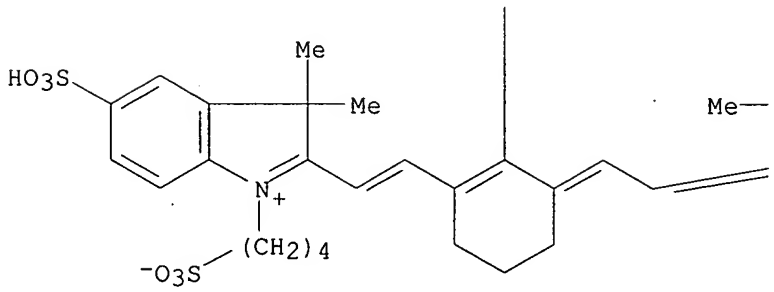
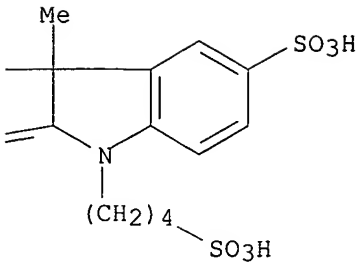


●3 Na

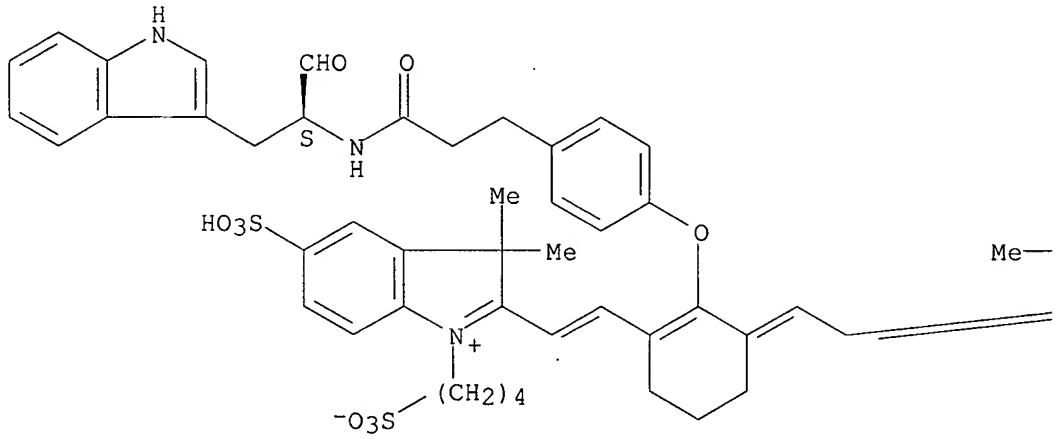
PAGE 2-B



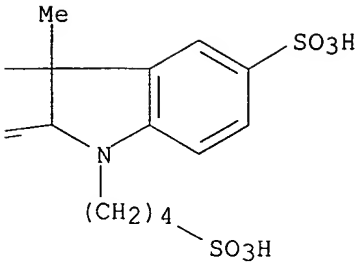
RN 607709-64-8 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[(1S)-1-formyl-2-(1H-indol-3-yl)ethyl]amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



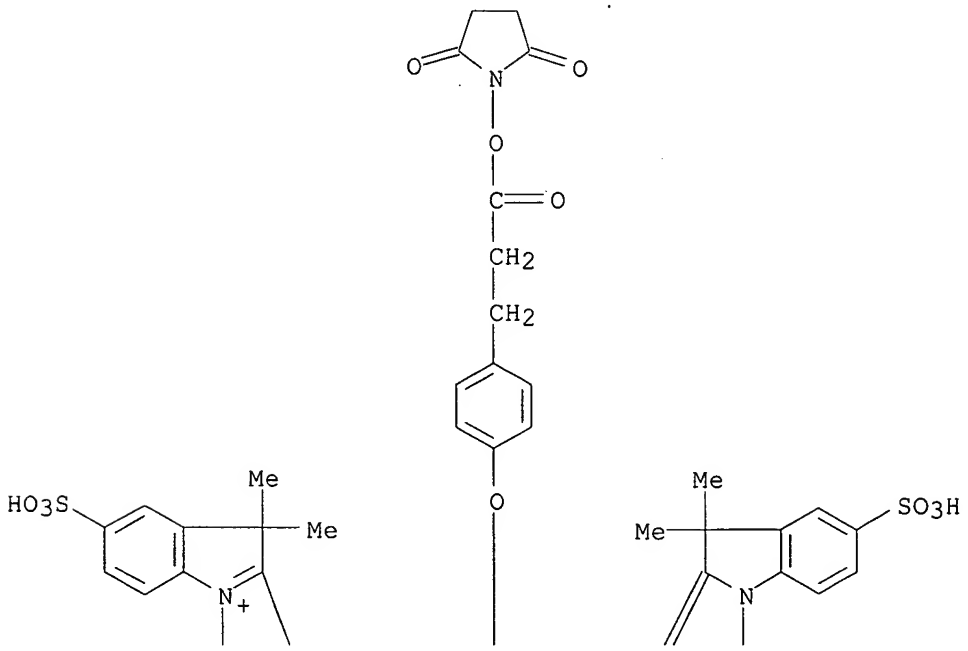
●3 Na

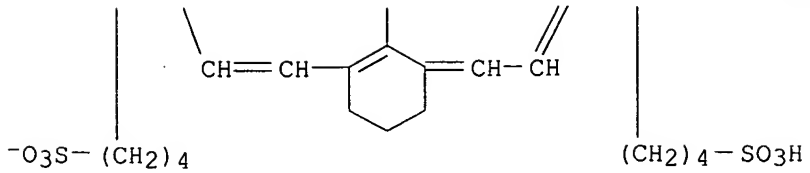


IT **398142-13-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(purification of IRDye78 conjugates by ion-pairing HPLC in relation to applications for near-IR fluorescence imaging)

RN 398142-13-7 HCAPLUS

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)





●3 Na

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:946293 HCAPLUS
DOCUMENT NUMBER: 138:19479
TITLE: Modified PSMA ligands for diagnosis and treatment of prostate cancer
INVENTOR(S): Frangioni, John V.
PATENT ASSIGNEE(S): Beth Israel Deaconess Medical Center, USA
SOURCE: PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002098885	A1	20021212	WO 2002-US21996	20020207 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2436408	AA	20021212	CA 2002-2436408	20020207 <--
EP 1363920	A1	20031126	EP 2002-761082	20020207 <--
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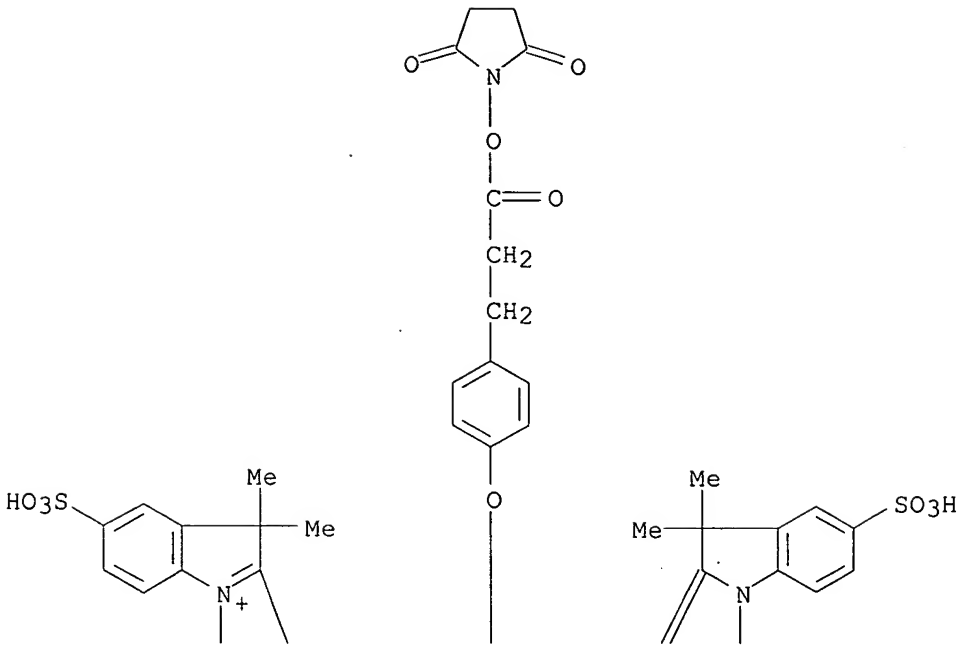
US 2004110723	A1	20040610	US 2002-71890	20020207 <--
US 6875886	B2	20050405		
JP 2005507857	T2	20050324	JP 2003-502006	20020207 <--
US 2004229845	A1	20041118	US 2004-869790	20040616 <--
PRIORITY APPLN. INFO.:			US 2001-267055P P	20010207 <--
			US 2002-71890 A1	20020207 <--
			WO 2002-US21996 W	20020207 <--

OTHER SOURCE(S): MARPAT 138:19479
IT **398142-13-7**, IRDye78
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(modified PSMA ligands for diagnosis and treatment of prostate cancer)
RN 398142-13-7 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



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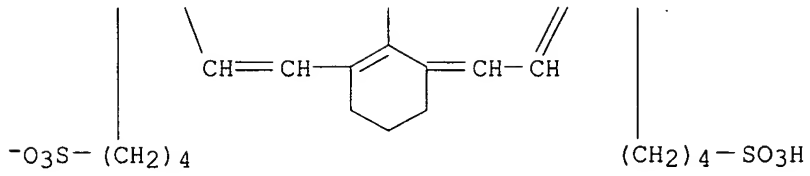


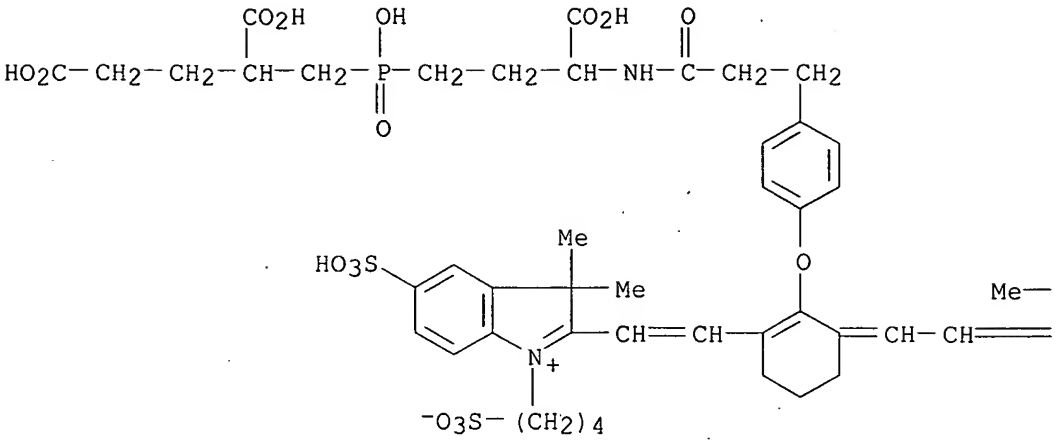
●3 Na

IT **477808-85-8 477808-86-9**
RL: DGN (Diagnostic use); BIOL (Biological study); USES (Uses)
(modified PSMA ligands for diagnosis and treatment of prostate cancer)

RN 477808-85-8 HCAPLUS

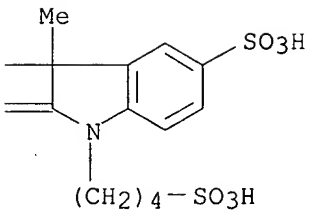
CN 3H-Indolium, 2-[2-[2-[4-[3-[[1-carboxy-3-[(2,4-dicarboxybutyl)hydroxyphosphinyl]propyl]amino]-3-oxopropyl]phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



●3 Na

PAGE 1-B

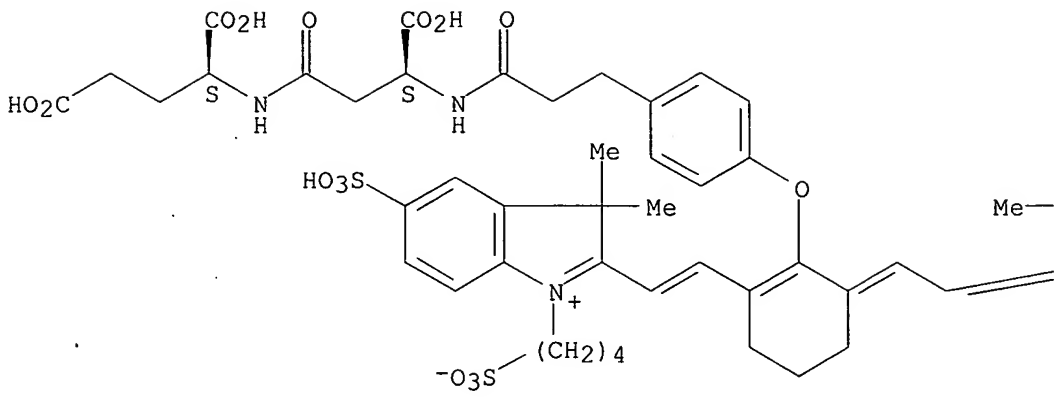


RN 477808-86-9 HCAPLUS

CN L-Glutamic acid, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-oxopropyl]-L-β-aspartyl-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

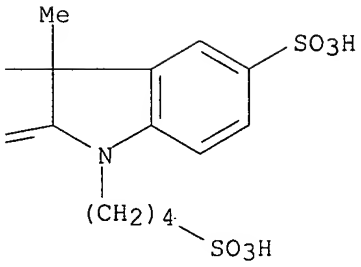
Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



●3 Na

PAGE 1-B



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:368351 HCAPLUS
DOCUMENT NUMBER: 136:366118
TITLE: Non-isotopic detection of osteoblastic activity in vivo using modified bisphosphonates
INVENTOR(S): Frangioni, John V.
PATENT ASSIGNEE(S): Beth Israel Deaconess Medical Center, USA
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002038190	A2	20020516	WO 2001-US51312	20011029 <--
WO 2002038190	A3	20020829		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002036683	A5	20020521	AU 2002-36683		20011029 <--
EP 1341557	A2	20030910	EP 2001-986230		20011029 <--
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US 6869593	B2	20050322			
PRIORITY APPLN. INFO.:			US 2000-244020P	P	20001027 <--
			WO 2001-US51312	W	20011029 <--

OTHER SOURCE(S): MARPAT 136:366118

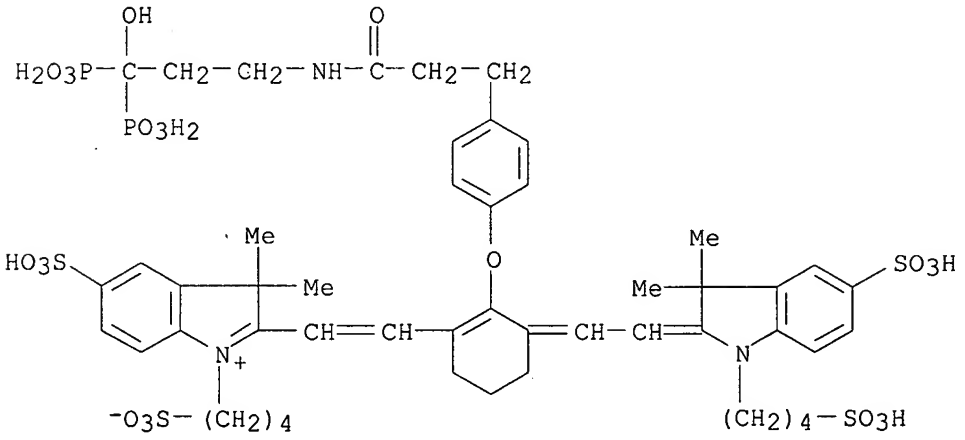
IT **424821-77-2P**

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Pam 78; nonisotopic detection of osteoblastic activity in vivo using modified bisphosphonates)

RN 424821-77-2 HCAPLUS

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(3-hydroxy-3,3-diphosphonopropyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, pentasodium salt (9CI) (CA INDEX NAME)



●5 Na

IT **398142-13-7**

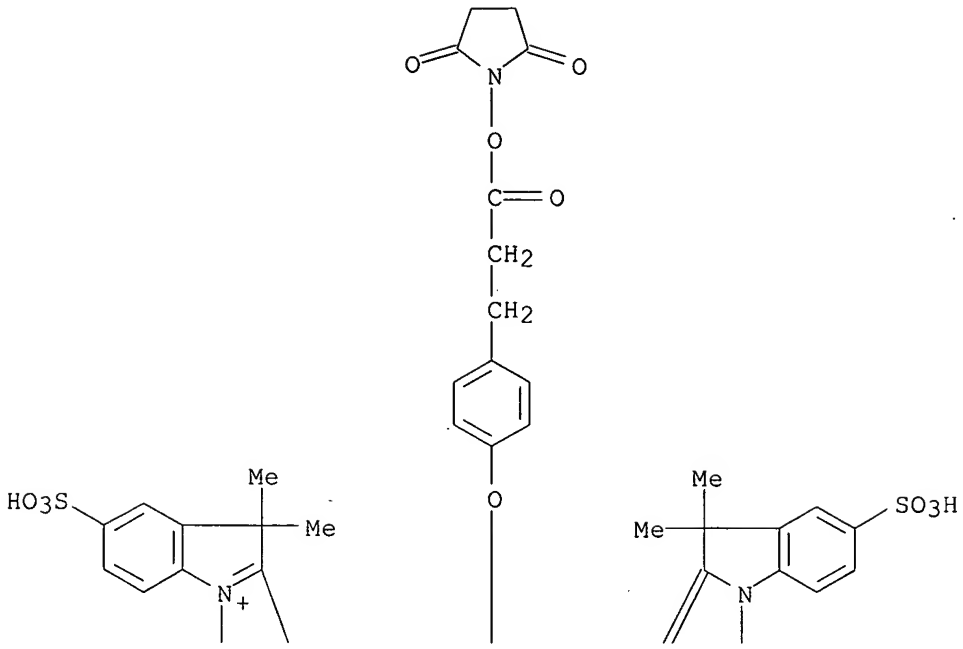
RL: RCT (Reactant); RACT (Reactant or reagent)

(nonisotopic detection of osteoblastic activity in vivo using modified bisphosphonates)

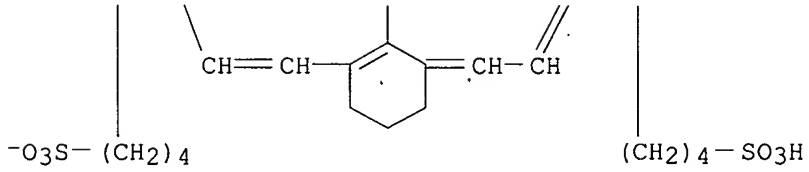
RN 398142-13-7 HCAPLUS

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



●3 Na

L32 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:314766 HCAPLUS
DOCUMENT NUMBER: 136:321680
TITLE: Indole and benzoindole derivatives as minimally invasive physiological function monitoring agents
INVENTOR(S): Achilefu, Samuel; Rajagopalan, Raghavan; Dorshow, Richard B.; Bugaj, Joseph E.
PATENT ASSIGNEE(S): Mallinckrodt Inc., USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002032421	A1	20020425	WO 2001-US31719	20011005 <--

WO 2002032421 C1 20020906
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 6733744	B1	20040511	US 2000-688946		20001016	
CA 2425701	AA	20020425	CA 2001-2425701		20011005	<--
AU 2002013100	A5	20020429	AU 2002-13100		20011005	<--
EP 1326602	A1	20030716	EP 2001-981460		20011005	<--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR						
JP 2004526669	T2	20040902	JP 2002-535659		20011005	<--
PRIORITY APPLN. INFO.:			US 2000-688946	A	20001016	<--
			WO 2001-US31719	W	20011005	<--

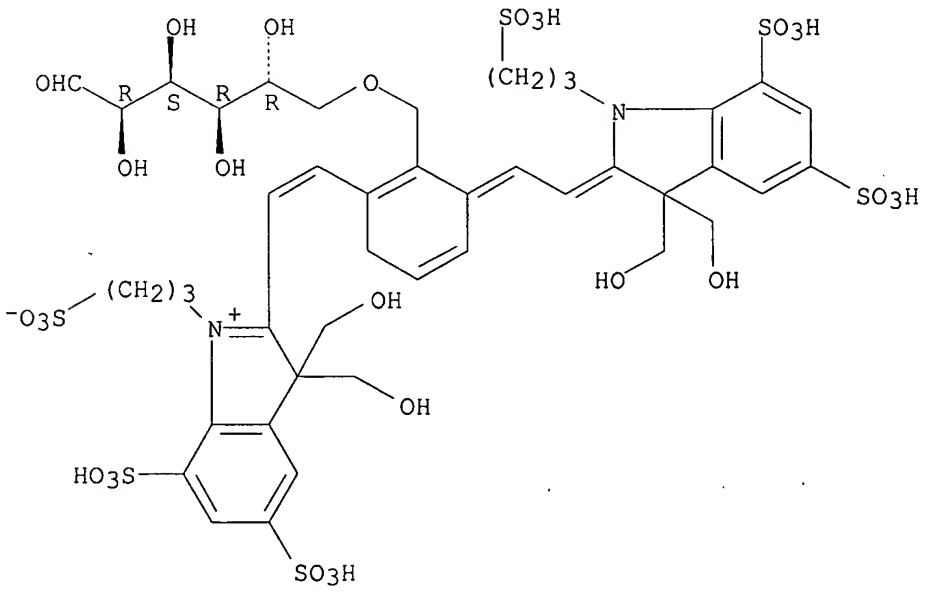
OTHER SOURCE(S): MARPAT 136:321680

IT **415727-03-6**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(indole and benzoindole derivs. as minimally invasive physiol. function monitoring agents)

RN 415727-03-6 HCAPLUS

CN D-Glucose, 6-O-[[2-[2-[3,3-bis(hydroxymethyl)-5,7-disulfo-1-(3-sulfopropyl)-3H-indolium-2-yl]ethenyl]-6-[[1,3-dihydro-3,3-bis(hydroxymethyl)-5,7-disulfo-1-(3-sulfopropyl)-2H-indol-2-ylidene]ethylidene]-1,4-cyclohexadien-1-yl]methyl]-, inner salt (9CI) (CA INDEX NAME)

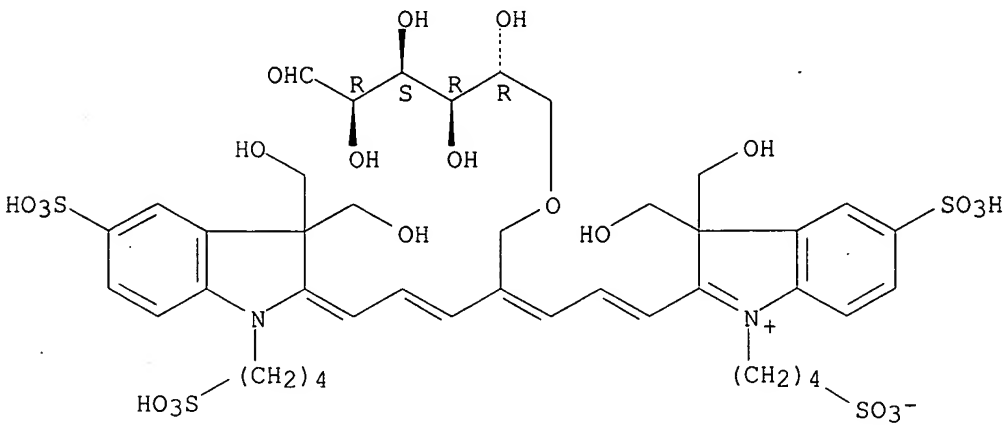
Absolute stereochemistry.
Double bond geometry unknown.



IT **415727-04-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(indole and benzoindole derivs. as minimally invasive physiol. function monitoring agents)

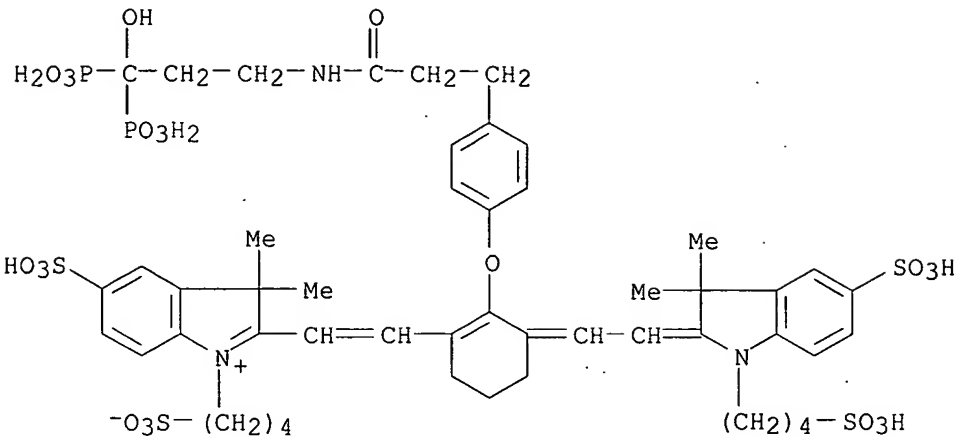
RN 415727-04-7 HCAPLUS
CN D-Glucose, 6-O-[5-[3,3-bis(hydroxymethyl)-5-sulfo-1-(4-sulfobutyl)-3H-indolium-2-yl]-2-[3-[1,3-dihydro-3,3-bis(hydroxymethyl)-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]-1-propenyl]-2,4-pentadienyl]-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



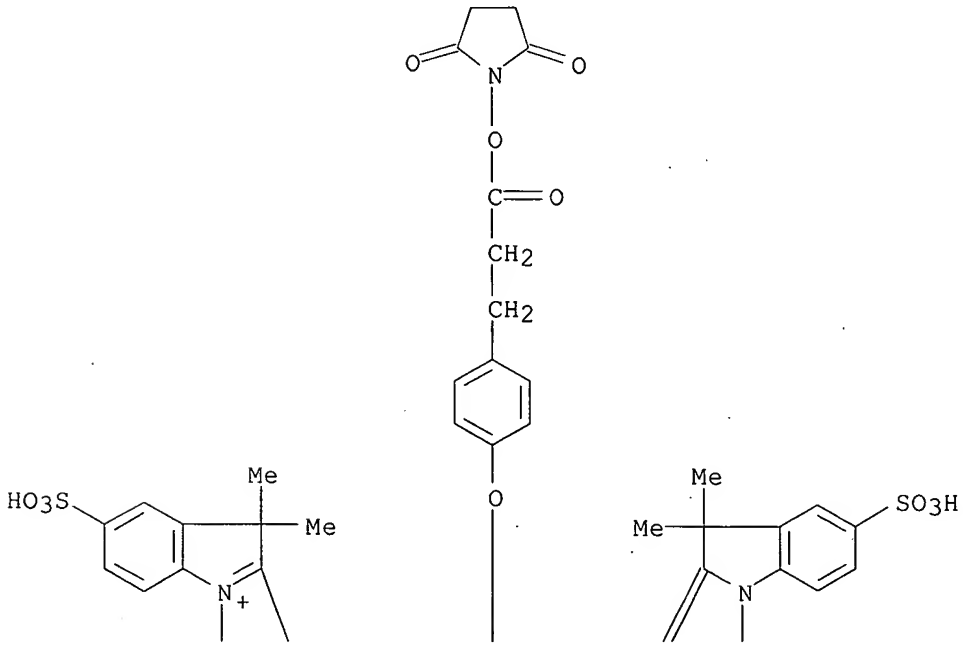
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

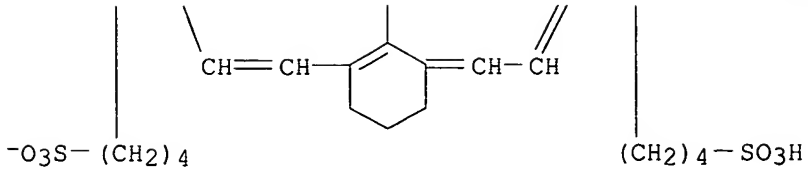
L32 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:909860 HCAPLUS
DOCUMENT NUMBER: 136:163487
TITLE: In vivo near-infrared fluorescence imaging of osteoblastic activity
AUTHOR(S): Zaheer, Atif; Lenkinski, Robert E.; Mahmood, Ashfaq; Jones, Alun G.; Cantley, Lewis C.; Frangioni, John V.
CORPORATE SOURCE: Department of Radiology, Beth Israel Deaconess Medical Center, Boston, MA, 02215, USA
SOURCE: Nature Biotechnology (**2001**), 19(12), 1148-1154
CODEN: NABIF9; ISSN: 1087-0156
PUBLISHER: Nature America Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **397858-89-8P**
RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(in vivo near-IR fluorescence imaging of osteoblastic activity)
RN 397858-89-8 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(3-hydroxy-3,3-diphosphonopropyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, heptasodium salt (9CI) (CA INDEX NAME)



●7 Na

IT **398142-13-7**, IRDye 78
RL: RCT (Reactant); RACT (Reactant or reagent)
(in vivo near-IR fluorescence imaging of osteoblastic activity)
RN 398142-13-7 HCAPLUS
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)





●3 Na

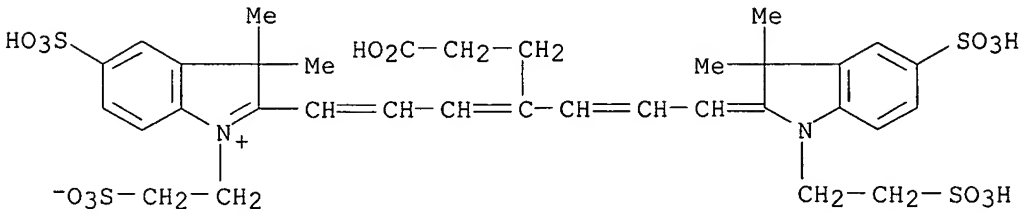
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 10 OF 13 USPATFULL on STN
ACCESSION NUMBER: 2004:328247 USPATFULL
TITLE: Hydrophilic, thiol-reactive cyanine dyes and conjugates thereof with biomolecules for fluorescence diagnosis
INVENTOR(S): Licha, Kai, Falkensee, GERMANY, FEDERAL REPUBLIC OF
Perlitz, Christin, Berlin, GERMANY, FEDERAL REPUBLIC OF

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2004260072	A1	20041223	
APPLICATION INFO.:	US 2004-762582	A1	20040123	(10)

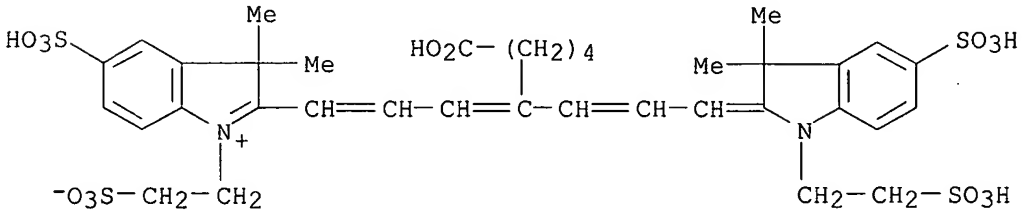
	NUMBER	DATE	
PRIORITY INFORMATION:	DE 2003-10302787	20030124	<--
	US 2003-443197P	20030129	(60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: MILLEN, WHITE, ZELANO & BRANIGAN, P.C., 2200 CLARENDON BLVD., SUITE 1400, ARLINGTON, VA, 22201
NUMBER OF CLAIMS: 34
EXEMPLARY CLAIM: 1
LINE COUNT: 1227
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **731862-91-2P 731862-98-9P 731863-01-7P**
731863-04-0P 731863-05-1P 731863-06-2P
731863-08-4P 731863-09-5P 731863-10-8P
(manufacture of hydrophilic, thiol-reactive cyanine dyes and conjugates thereof with biomols. for fluorescence diagnosis)
RN 731862-91-2 USPATFULL
CN 3H-Indolium, 2-[4-(2-carboxyethyl)-7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



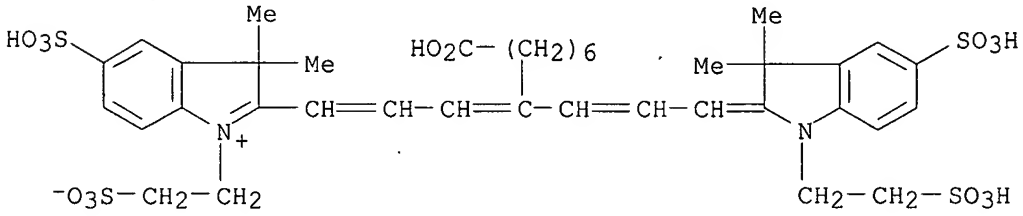
●3 Na

RN 731862-98-9 USPATFULL
CN 3H-Indolium, 2-[8-carboxy-4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-1,3-octadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



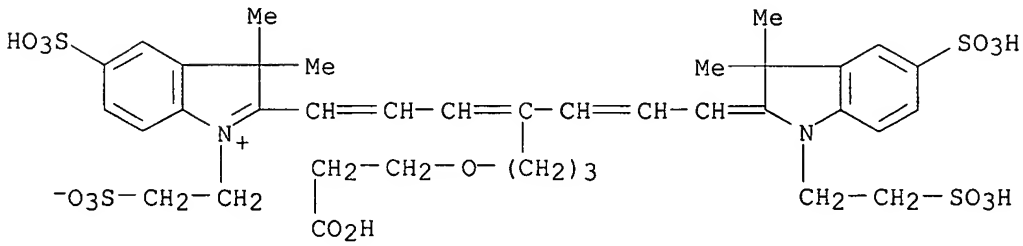
●3 Na

RN 731863-01-7 USPATFULL
CN 3H-Indolium, 2-[10-carboxy-4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-1,3-decadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



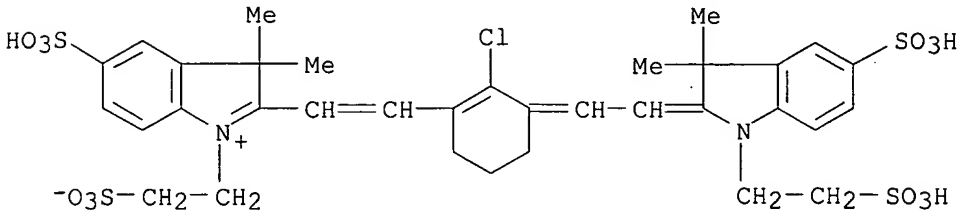
●3 Na

RN 731863-04-0 USPATFULL
CN 3H-Indolium, 2-[4-[3-(2-carboxyethoxy)propyl]-7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



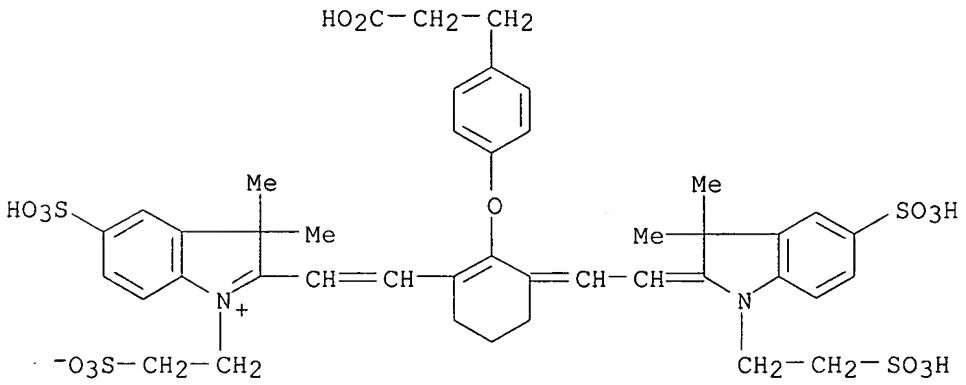
●3 Na

RN 731863-05-1 USPATFULL
CN 3H-Indolium, 2-[2-[2-chloro-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



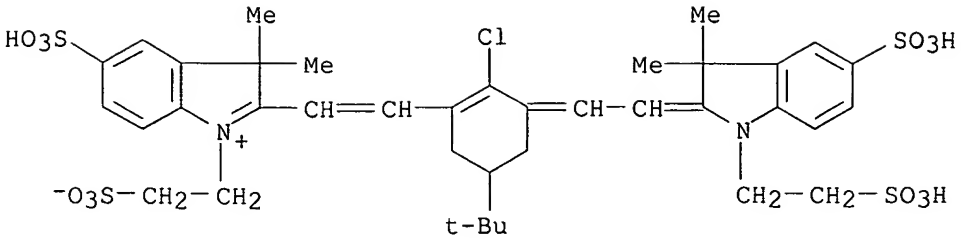
●3 Na

RN 731863-06-2 USPATFULL
CN 3H-Indolium, 2-[2-[2-[4-(2-carboxyethyl)phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



●3 Na

RN 731863-08-4 USPATFULL
CN 3H-Indolium, 2-[2-[2-chloro-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-5-(1,1-dimethylethyl)-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



●3 Na

RN 731863-09-5 USPATFULL
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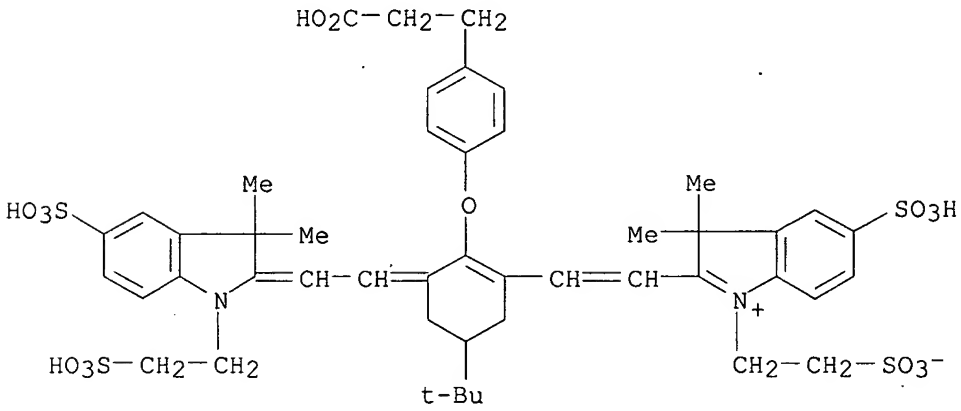
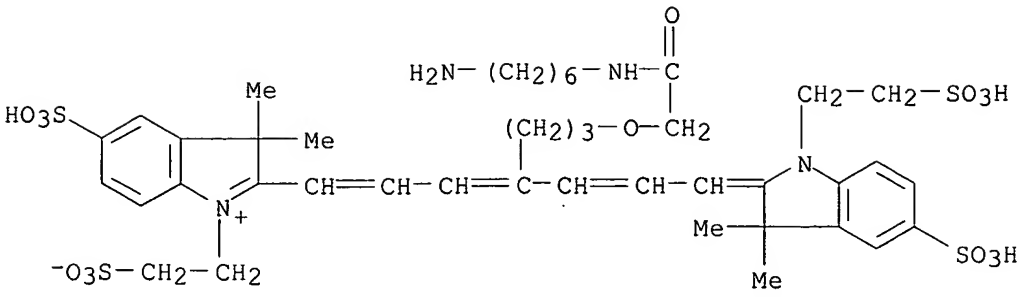


●3 Na

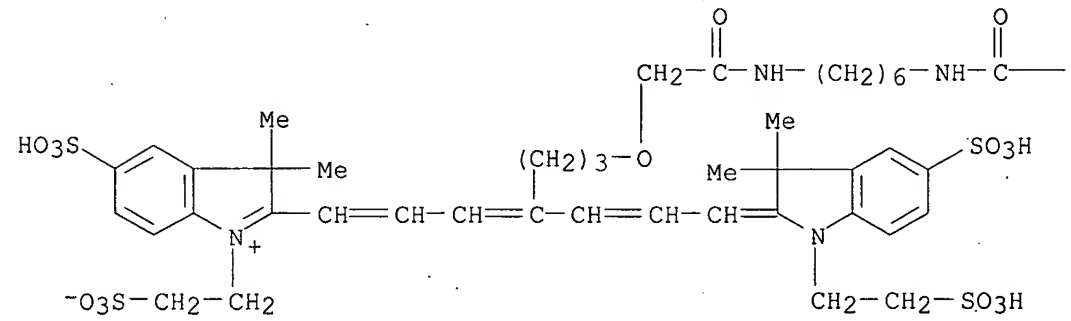
RN 731863-10-8 USPATFULL
CN 3H-Indolium, 2-[4-[3-[2-[(6-aminohexyl)amino]-2-oxoethoxy]propyl]-7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



●3 Na

IT **731862-87-6P**
(manufacture of hydrophilic, thiol-reactive cyanine dyes and conjugates thereof with biomols. for fluorescence diagnosis)
RN 731862-87-6 USPATFULL
CN 3H-Indolium, 2-[4-[3-[2-[[6-[(bromoacetyl)amino]hexyl]amino]-2-oxoethoxy]propyl]-7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



●3 Na

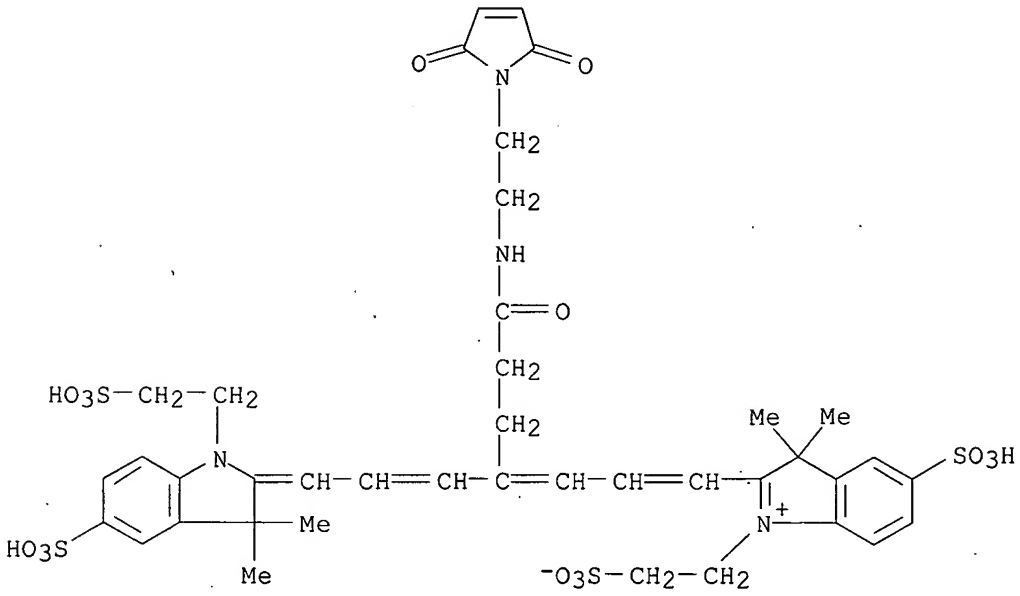
PAGE 1-B

— CH_2Br

IT **731862-71-8P 731862-72-9P 731862-73-0P**
731862-74-1P 731862-75-2P 731862-76-3P
731862-77-4P 731862-78-5P 731862-79-6P
731862-80-9P 731862-81-0P 731862-82-1P
731862-83-2P 731862-84-3P 731862-85-4P
731862-86-5P 731862-88-7P
(manufacture of hydrophilic, thiol-reactive cyanine dyes and conjugates thereof with biomols. for fluorescence diagnosis)
RN 731862-71-8 USPATFULL
CN 3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-

indol-2-ylidene]-4-[3-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-3-oxopropyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

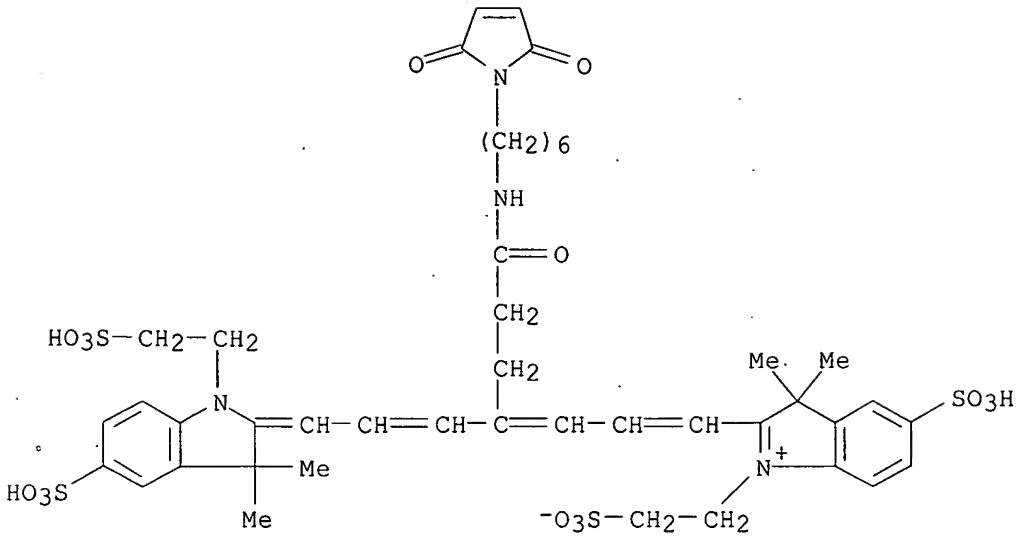


PAGE 2-A

●3 Na

RN 731862-72-9 USPATFULL
CN 3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-4-[3-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexyl]amino]-3-oxopropyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

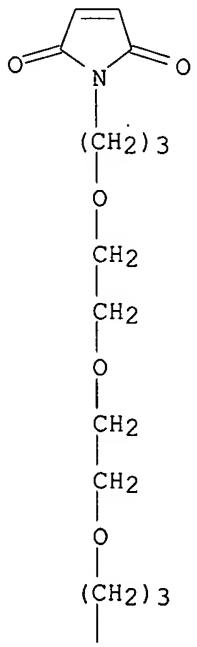


PAGE 2-A

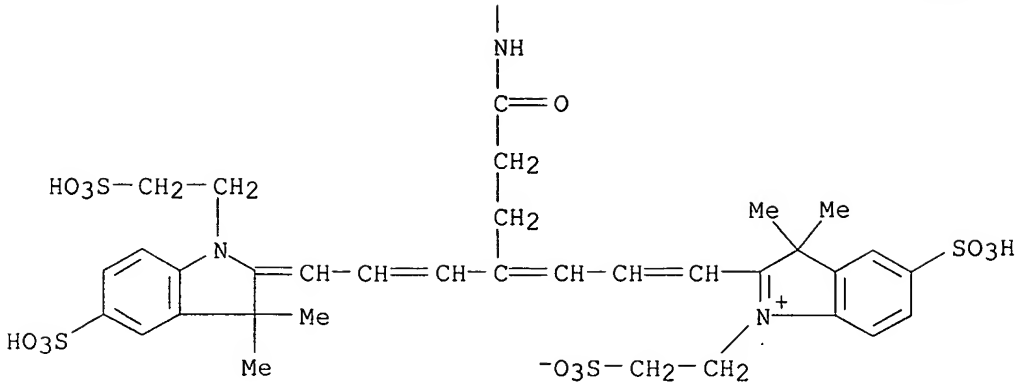
●3 Na

RN 731862-73-0 USPATFULL
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-21-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-7-oxo-12,15,18-trioxa-8-azaheneicosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



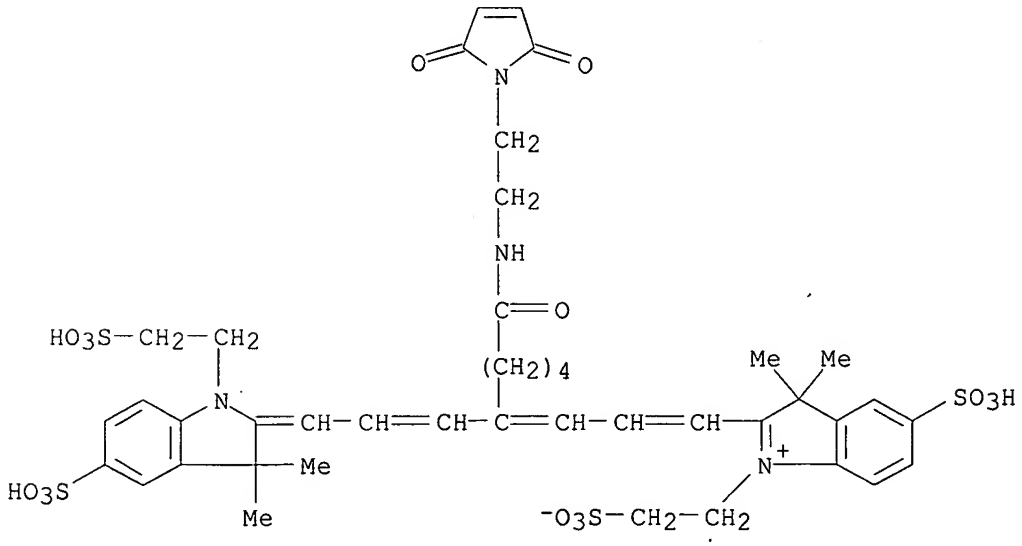
PAGE 2-A



●3 Na

RN 731862-74-1 USPATFULL
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-9-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-9-oxo-1,3-nonadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

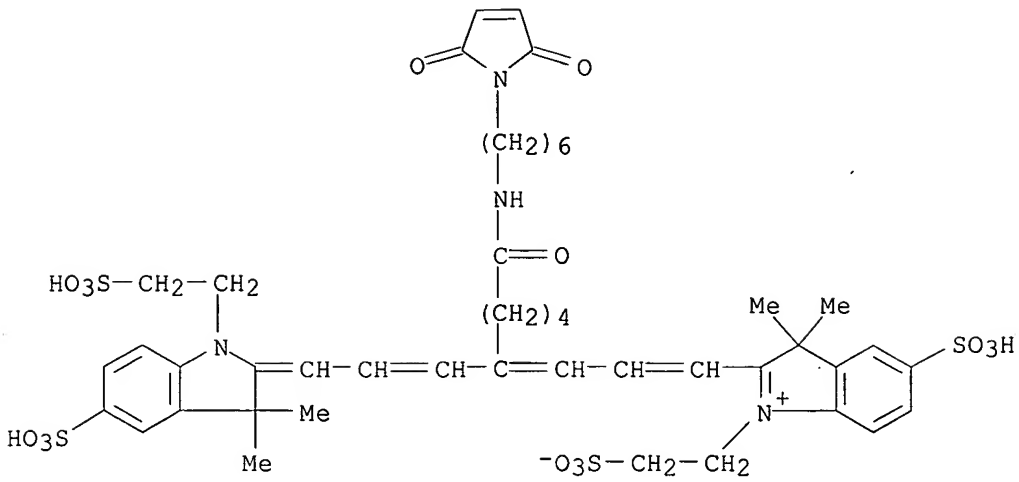
PAGE 1-A



PAGE 2-A

●3 Na

RN 731862-75-2 USPATFULL
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-9-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexyl]amino]-9-oxo-1,3-nonadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



●3 Na

RN 731862-76-3 USPATFULL
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-23-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-9-oxo-14,17,20-trioxa-10-azatricosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

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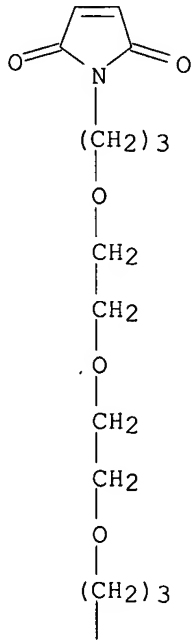
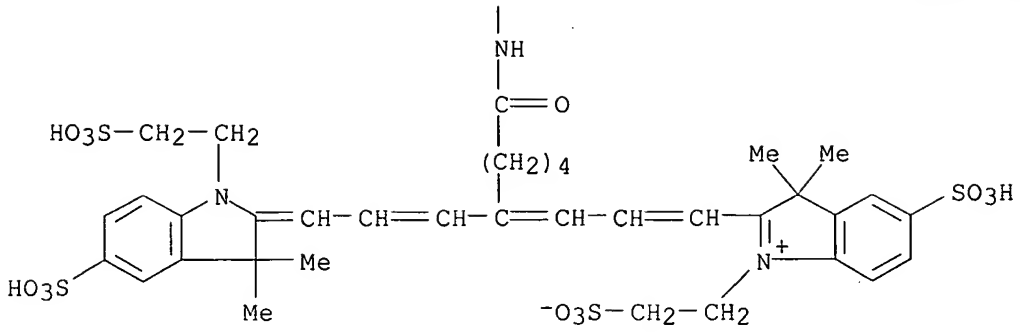


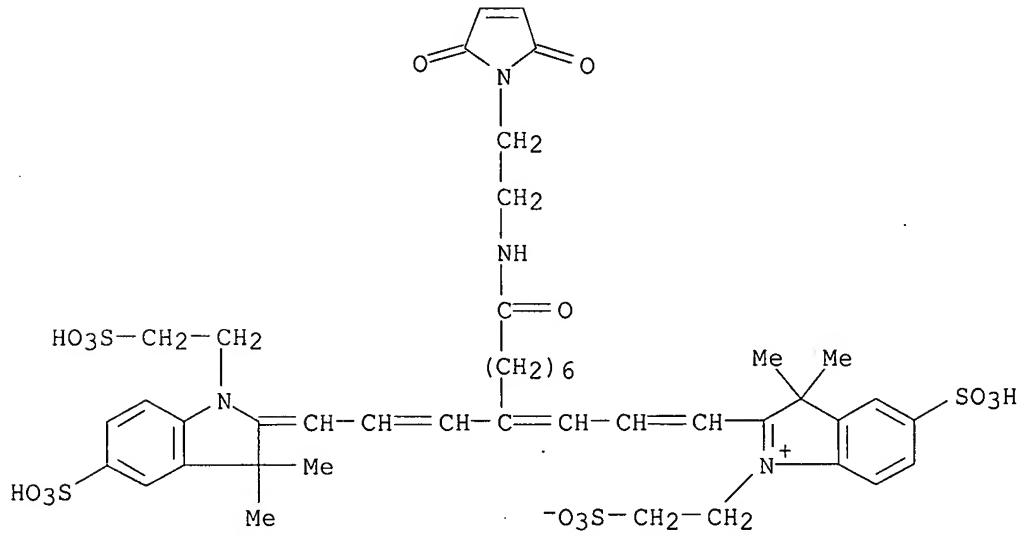
PAGE 2-A



●3 Na

RN 731862-77-4 USPATFULL
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-11-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-11-oxo-1,3-undecadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



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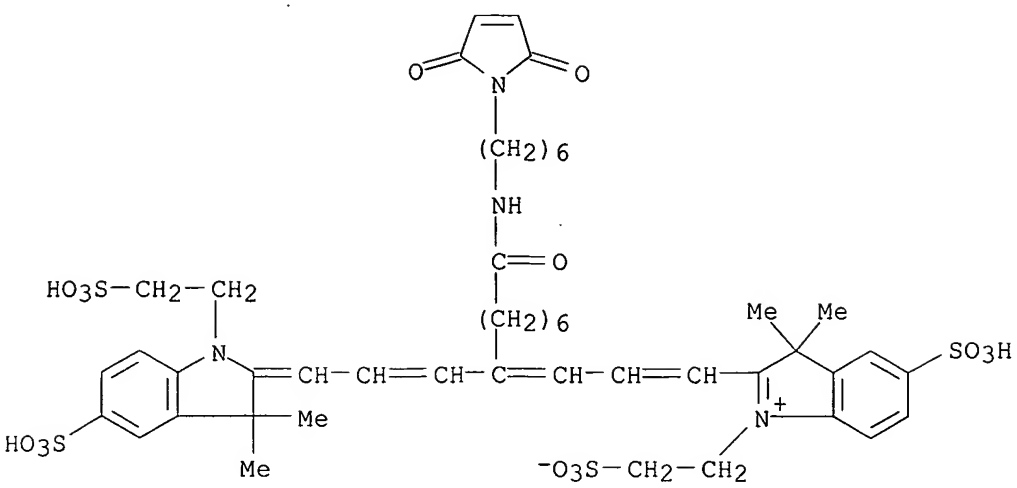
●3 Na

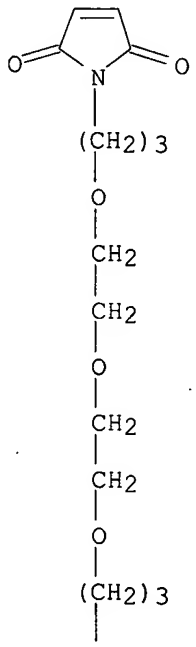
RN 731862-78-5 USPATFULL
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-11-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexyl]amino]-11-oxo-1,3-undecadienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



●3 Na

RN 731862-79-6 USPATFULL

CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-25-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-11-oxo-16,19,22-trioxa-12-azapentacosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)



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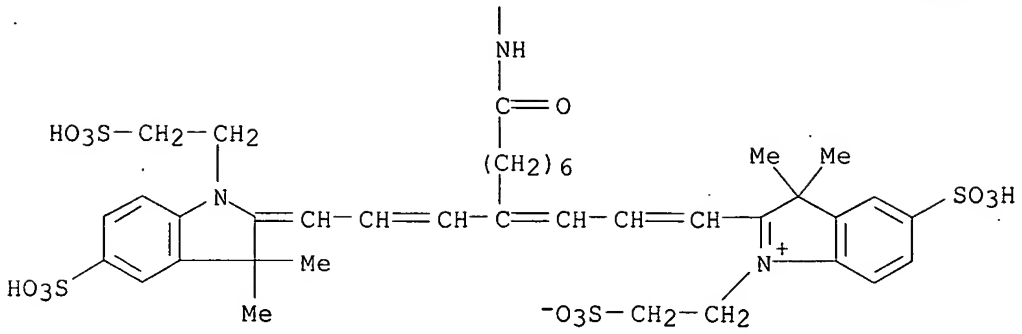
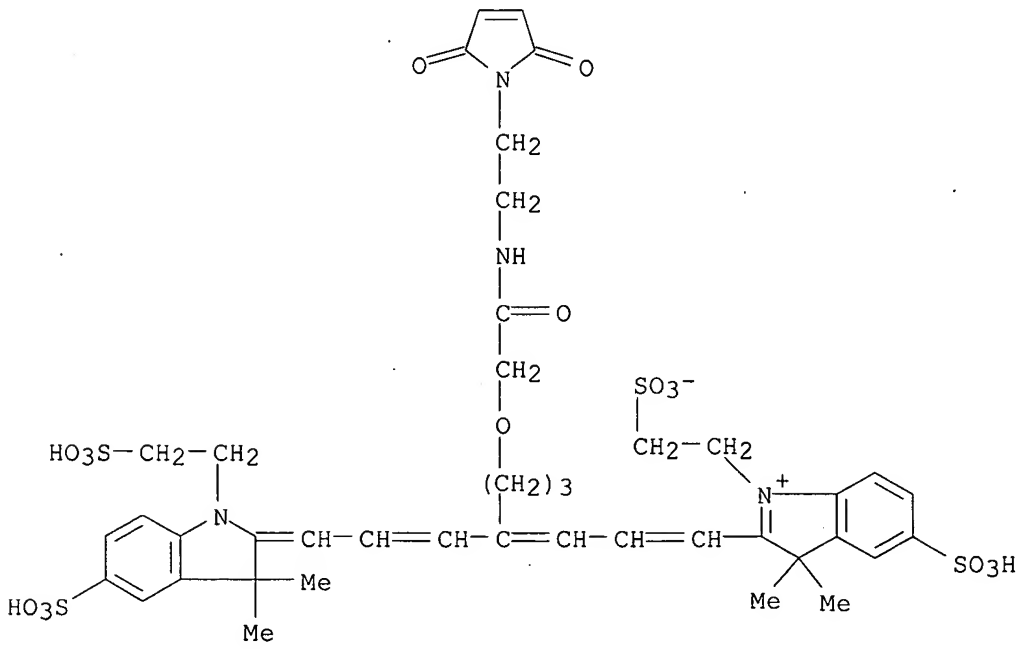


●3 Na

RN 731862-80-9 USPATFULL
CN 3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-4-[3-[2-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-2-oxoethoxy]propyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



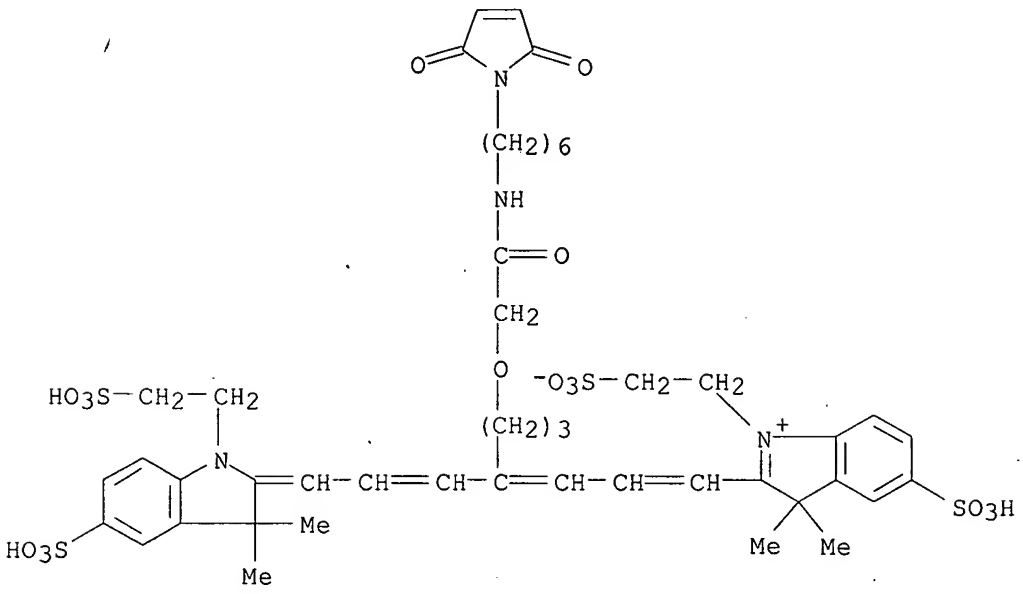
PAGE 2-A

●3 Na

RN 731862-81-0 USPATFULL
CN 3H-Indolium, 2-[7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-4-[3-[2-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-

yl)hexyl]amino]-2-oxoethoxy]propyl]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



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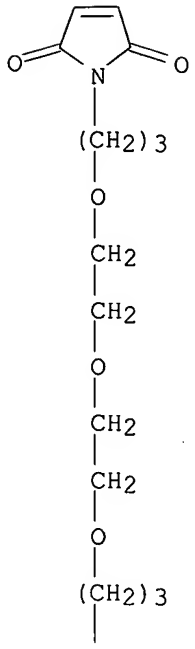
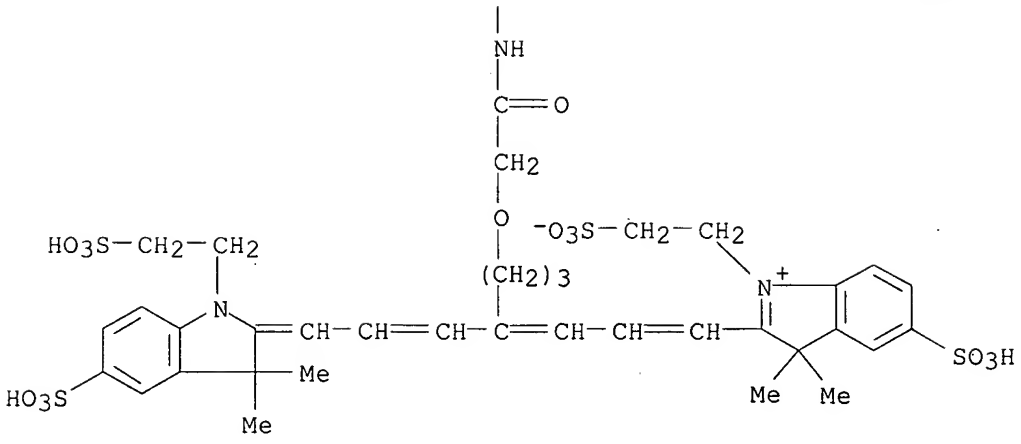
●3 Na

RN 731862-82-1 USPATFULL
CN 3H-Indolium, 2-[4-[3-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1-propenyl]-24-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-10-oxo-8,15,18,21-tetraoxa-11-azatetracosa-1,3-dien-1-yl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



●3 Na

RN 731862-83-2 USPATFULL
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

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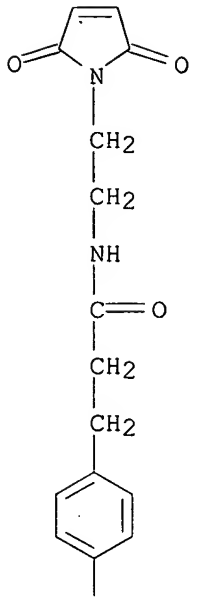
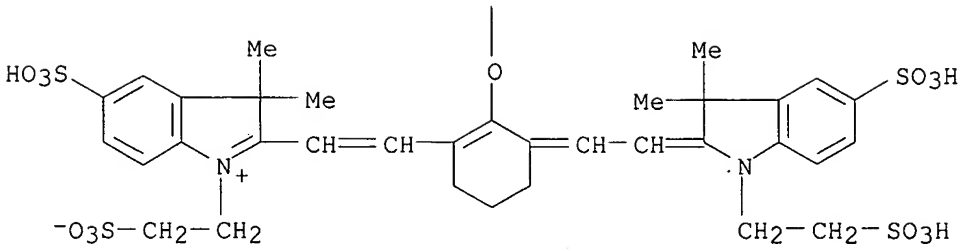


PAGE 2-A

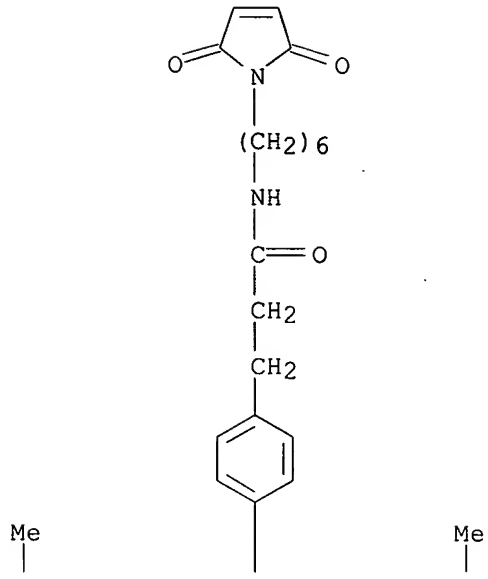


●3 Na

RN 731862-84-3 USPATFULL

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexyl]amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



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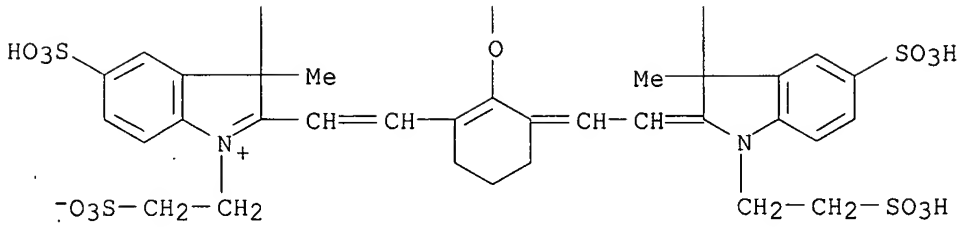
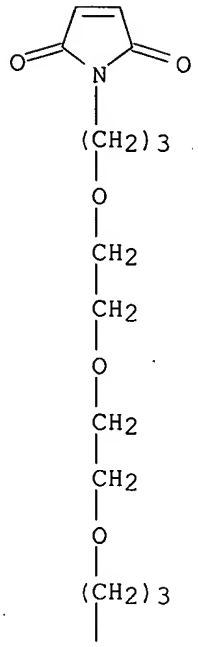


●3 Na

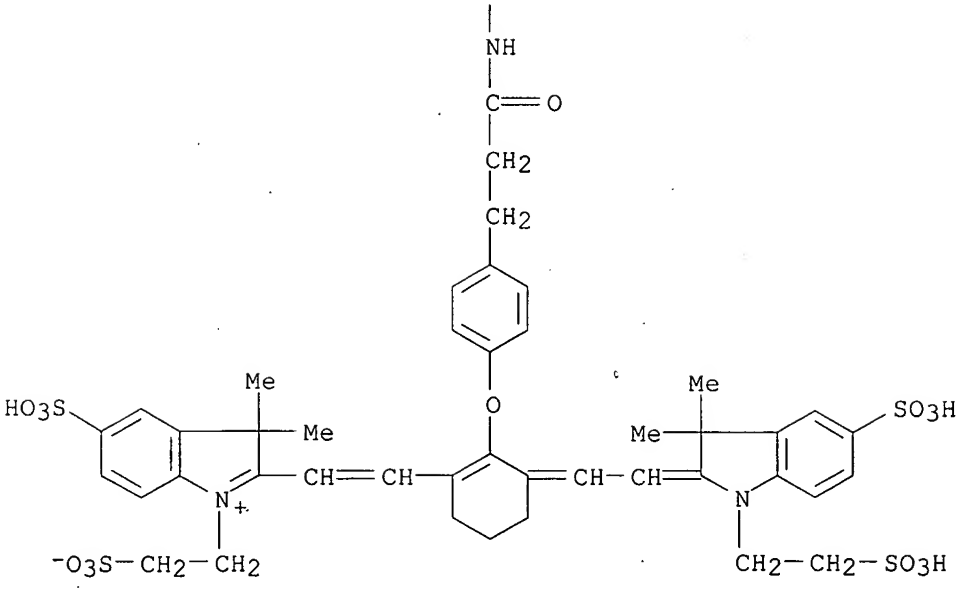
RN 731862-85-4 USPATFULL

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[17-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-3-oxo-8,11,14-trioxa-4-azaheptadec-1-yl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



PAGE 3-A

●3 Na

RN 731862-86-5 USPATFULL
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]amino]-3-oxopropyl]phenoxy]-5-(1,1-dimethylethyl)-1-

cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

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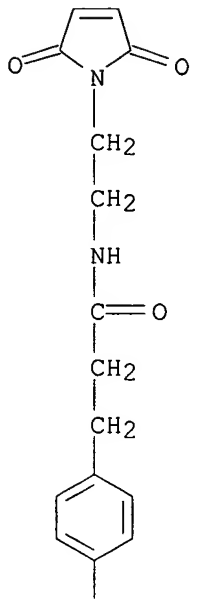
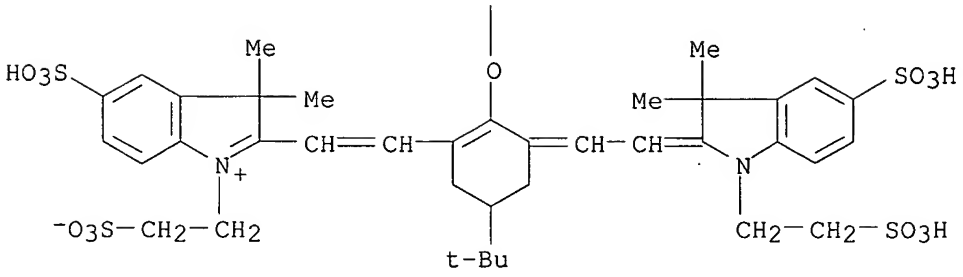


PAGE 2-A



●3 Na

RN 731862-88-7 USPATFULL

CN 3H-Indolium, 2-[4-[3-[[3-[(bromoacetyl)amino]propyl]amino]-3-oxopropyl]-7-[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-2H-indol-2-ylidene]-1,3,5-heptatrienyl]-3,3-dimethyl-5-sulfo-1-(2-sulfoethyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

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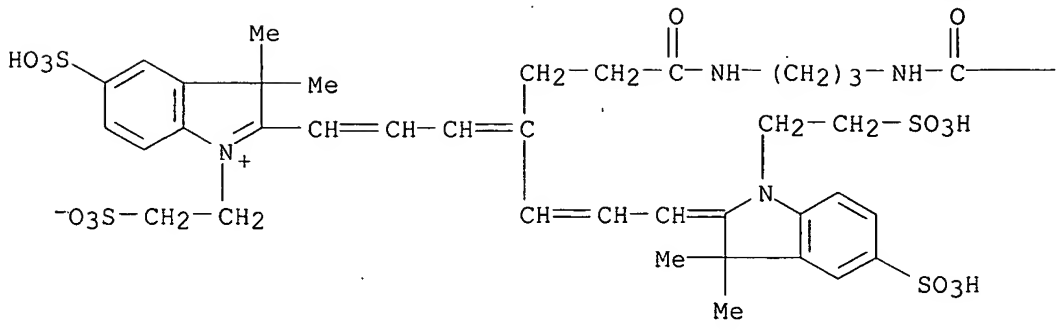
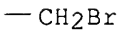


●3 Na

PAGE 1-B



L32 ANSWER 11 OF 13 USPATFULL on STN

ACCESSION NUMBER:	2004:292756 USPATFULL
TITLE:	Modified PSMA ligands and uses related thereto
INVENTOR(S):	Frangioni, John V., Wayland, MA, UNITED STATES
PATENT ASSIGNEE(S):	Beth Israel Deaconess Medical Center, Boston, MA (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004229845	A1	20041118
APPLICATION INFO.:	US 2004-869790	A1	20040616 (10)

RELATED APPLN. INFO.: Continuation of Ser. No. US 2002-71890, filed on 7 Feb 2002, PENDING

	NUMBER	DATE	
PRIORITY INFORMATION:	US 2001-267055P	20010207 (60)	<--

DOCUMENT TYPE:	Utility
FILE SEGMENT:	APPLICATION
LEGAL REPRESENTATIVE:	ROPES & GRAY LLP, ONE INTERNATIONAL PLACE, BOSTON, MA, 02110-2624
NUMBER OF CLAIMS:	66
EXEMPLARY CLAIM:	1
NUMBER OF DRAWINGS:	11 Drawing Page(s)
LINE COUNT:	1759

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **398142-13-7**, IRDye78
(modified PSMA ligands for diagnosis and treatment of prostate cancer)

RN 398142-13-7 USPATFULL

CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

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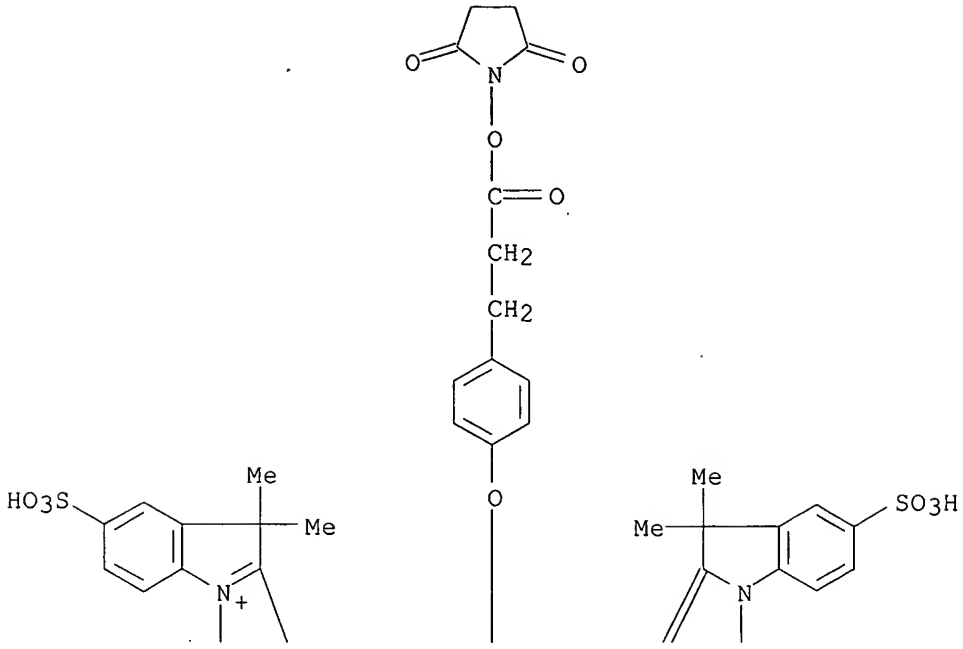
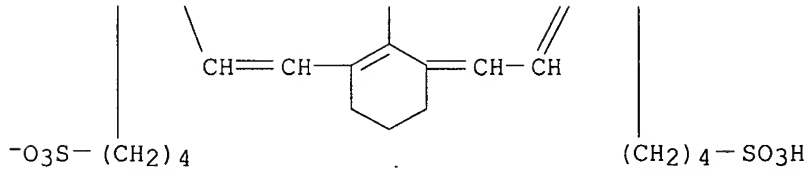


PAGE 2-A



●3 Na

IT **477808-85-8 477808-86-9**
(modified PSMA ligands for diagnosis and treatment of prostate cancer)
RN 477808-85-8 USPATFULL
CN 3H-Indolium, 2-[2-[2-[4-[3-[[1-carboxy-3-[(2,4-dicarboxybutyl)hydroxyphosphinyl]propyl]amino]-3-oxopropyl]phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

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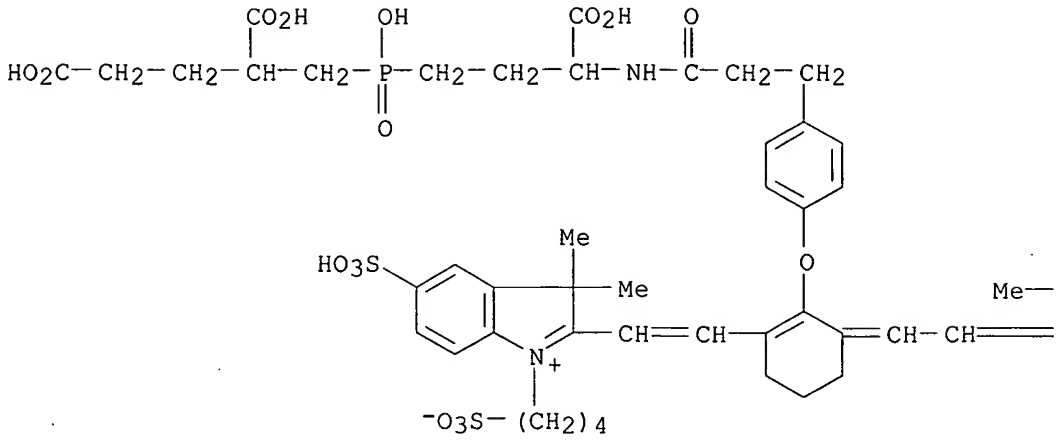

●3 Na

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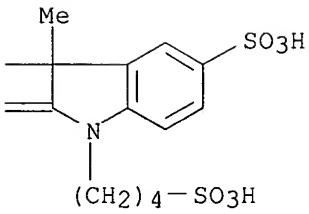

RN 477808-86-9 USPATFULL

CN L-Glutamic acid, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-oxopropyl]-L-β-aspartyl-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

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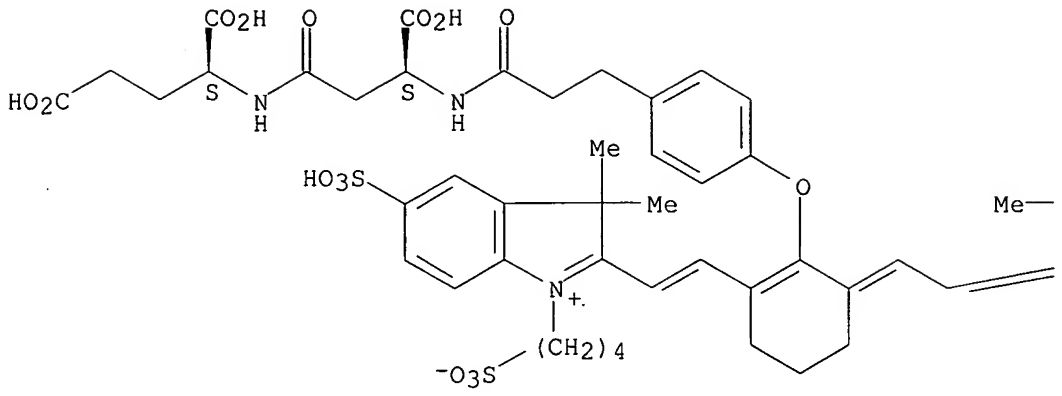

●3 Na

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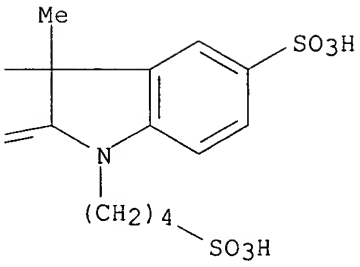

L32 ANSWER 12 OF 13 USPATFULL on STN

ACCESSION NUMBER:	2004:145051 USPATFULL			
TITLE:	MODIFIED PSMA LIGANDS AND USES RELATED THERETO			
INVENTOR(S):	Frangioni, John V., Wayland, MA, UNITED STATES			
	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2004110723	A1	20040610	
	US 6875886	B2	20050405	
APPLICATION INFO.:	US 2002-71890	A1	20020207	(10)
	NUMBER		DATE	
PRIORITY INFORMATION:	US 2001-267055P		20010207 (60)	<--
DOCUMENT TYPE:	Utility			
FILE SEGMENT:	APPLICATION			
LEGAL REPRESENTATIVE:	ROPES & GRAY LLP, ONE INTERNATIONAL PLACE, BOSTON, MA, 02110-2624			
NUMBER OF CLAIMS:	66			
EXEMPLARY CLAIM:	1			

NUMBER OF DRAWINGS: 11 Drawing Page(s)
LINE COUNT: 1757
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **398142-13-7**, IRDye78
(modified PSMA ligands for diagnosis and treatment of prostate cancer)
RN 398142-13-7 USPATFULL
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(2,5-dioxo-1-pyrrolidinyl)oxy]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

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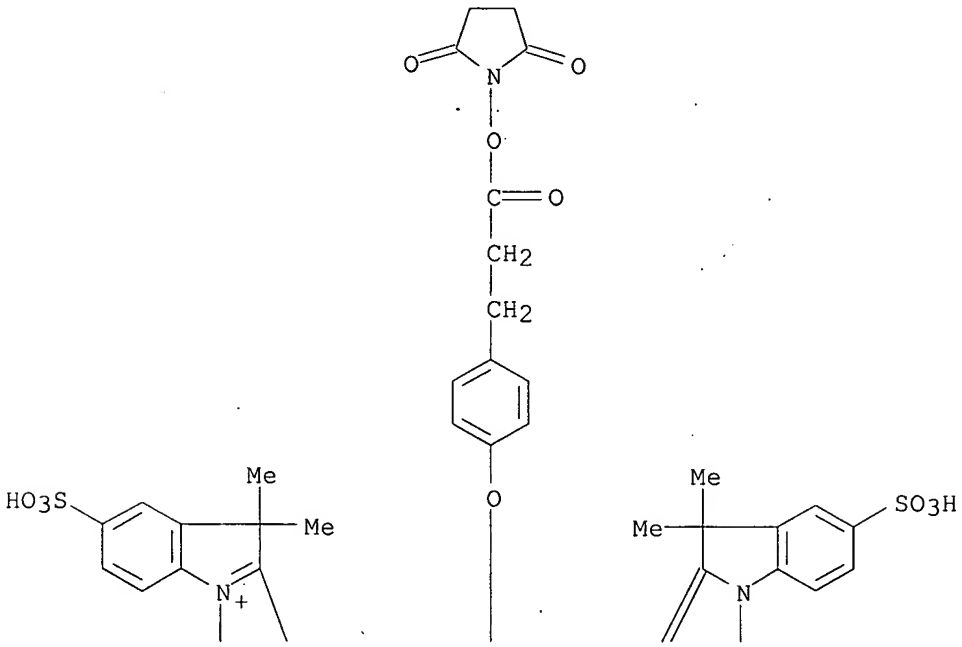

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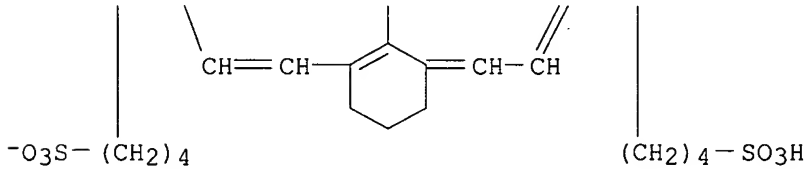

● 3 Na

IT **477808-85-8 477808-86-9**
(modified PSMA ligands for diagnosis and treatment of prostate cancer)
RN 477808-85-8 USPATFULL
CN 3H-Indolium, 2-[2-[2-[4-[3-[[1-carboxy-3-[(2,4-dicarboxybutyl)hydroxyphosphinyl]propyl]amino]-3-oxopropyl]phenoxy]-3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

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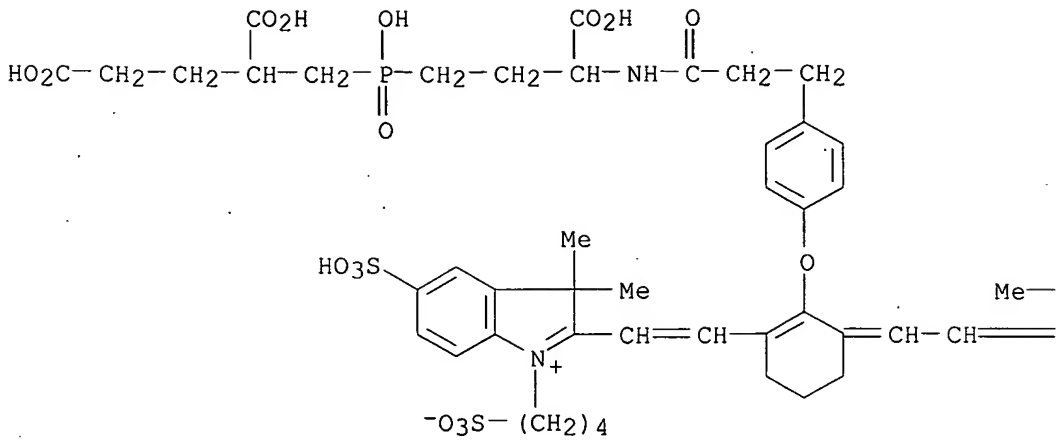
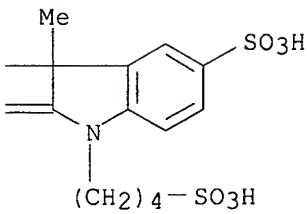


●3 Na

PAGE 1-B

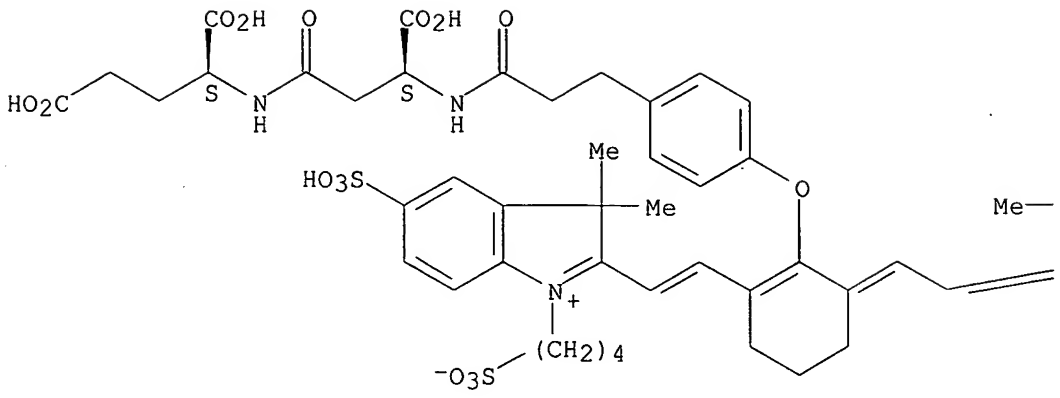


RN 477808-86-9 USPATFULL

CN L-Glutamic acid, N-[3-[4-[[6-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[2-[3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-3H-indolium-2-yl]ethenyl]-1-cyclohexen-1-yl]oxy]phenyl]-1-oxopropyl]-L-β-aspartyl-, inner salt, trisodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



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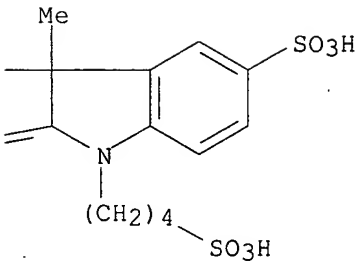
PAGE 1-B



L32 ANSWER 13 OF 13 USPATFULL on STN

ACCESSION NUMBER: 2004:38075 USPATFULL

TITLE: Non-isotopic detection of osteoblastic activity in vivo using modified bisphosphonates

INVENTOR(S): Frangioni, John V., Wayland, MA, UNITED STATES

PATENT ASSIGNEE(S): Beth Israel Deaconess Medical Center, of the entire inerst. (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004028611	A1	20040212
	US 6869593	B2	20050322
APPLICATION INFO.:	US 2003-424572	A1	20030425 (10)

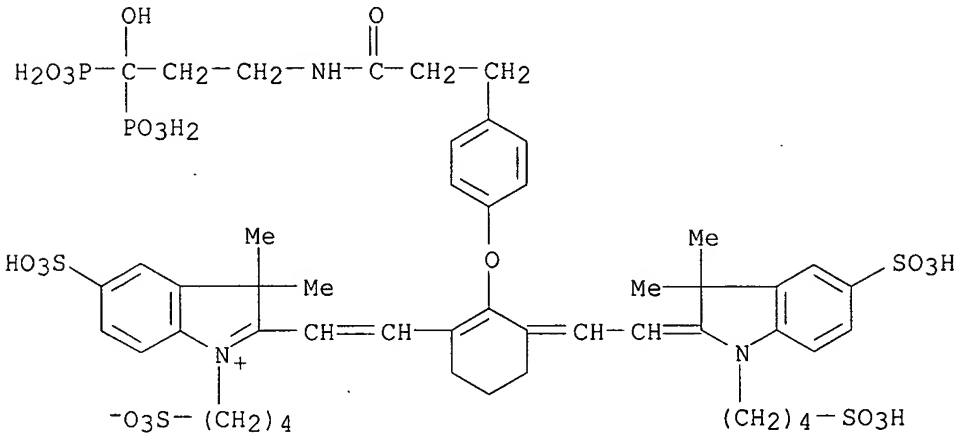
RELATED APPLN. INFO.: Continuation of Ser. No. WO 2001-US51312, filed on 29 Oct 2001, PENDING

	NUMBER	DATE	
PRIORITY INFORMATION:	US 2000-244020P	20001027 (60)	<--

DOCUMENT TYPE: Utility

FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: HAMILTON, BROOK, SMITH & REYNOLDS, P.C., 530 VIRGINIA ROAD, P.O. BOX 9133, CONCORD, MA, 01742-9133
NUMBER OF CLAIMS: 28
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 7 Drawing Page(s)
LINE COUNT: 1313
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **424821-77-2P**
(Pam 78; nonisotopic detection of osteoblastic activity in vivo using modified bisphosphonates)
RN 424821-77-2 USPATFULL
CN 3H-Indolium, 2-[2-[3-[[1,3-dihydro-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-2H-indol-2-ylidene]ethylidene]-2-[4-[3-[(3-hydroxy-3,3-diphosphonopropyl)amino]-3-oxopropyl]phenoxy]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-5-sulfo-1-(4-sulfobutyl)-, inner salt, pentasodium salt (9CI) (CA INDEX NAME)



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IT **398142-13-7**
(nonisotopic detection of osteoblastic activity in vivo using modified bisphosphonates)
RN 398142-13-7 USPATFULL
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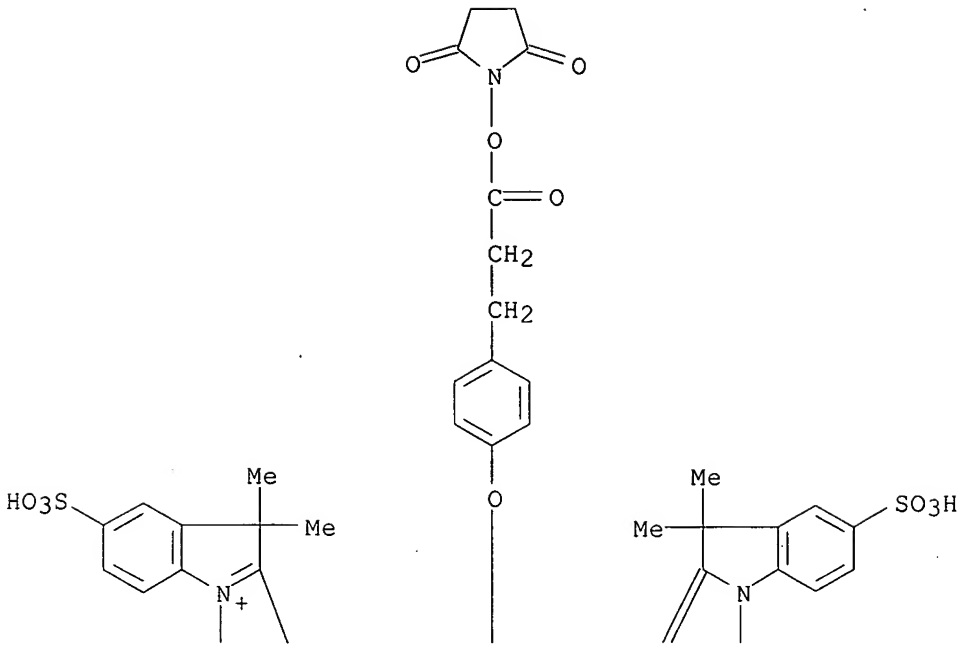
PAGE 1-A



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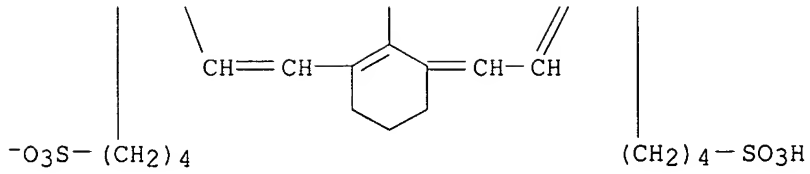

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